Fig. 1

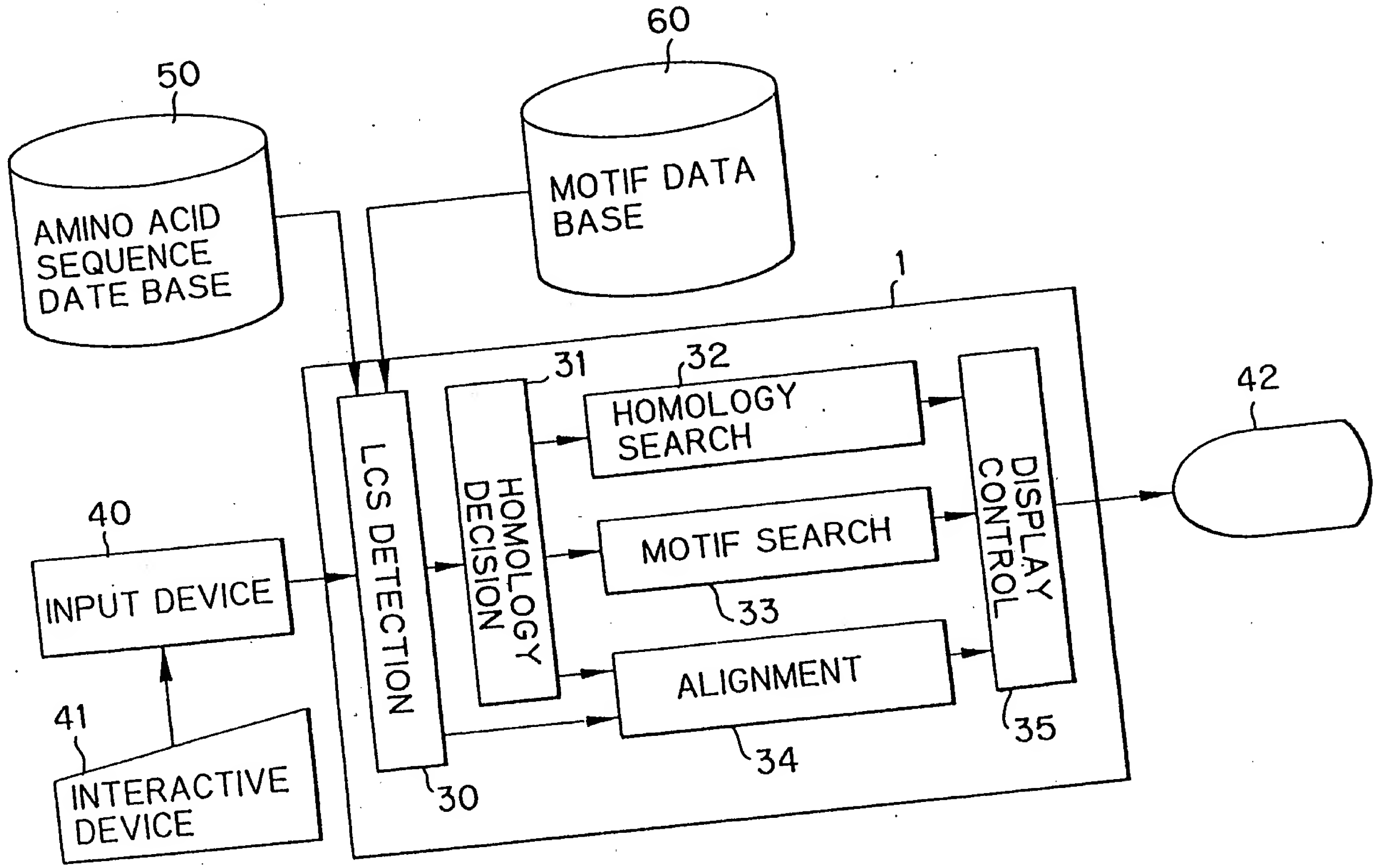

60
MOTIF DATA BASE
50
AMINO ACID SEQUENCE DATE BASE
1
31
32
HOMOLOGY SEARCH
LCS DETECTION
HOMOLOGY DECISION
MOTIF SEARCH
33
ALIGNMENT
34
DISPLAY CONTROL
35
30
42
40
INPUT DEVICE
41
INTERACTIVE DEVICE

Fig. 2

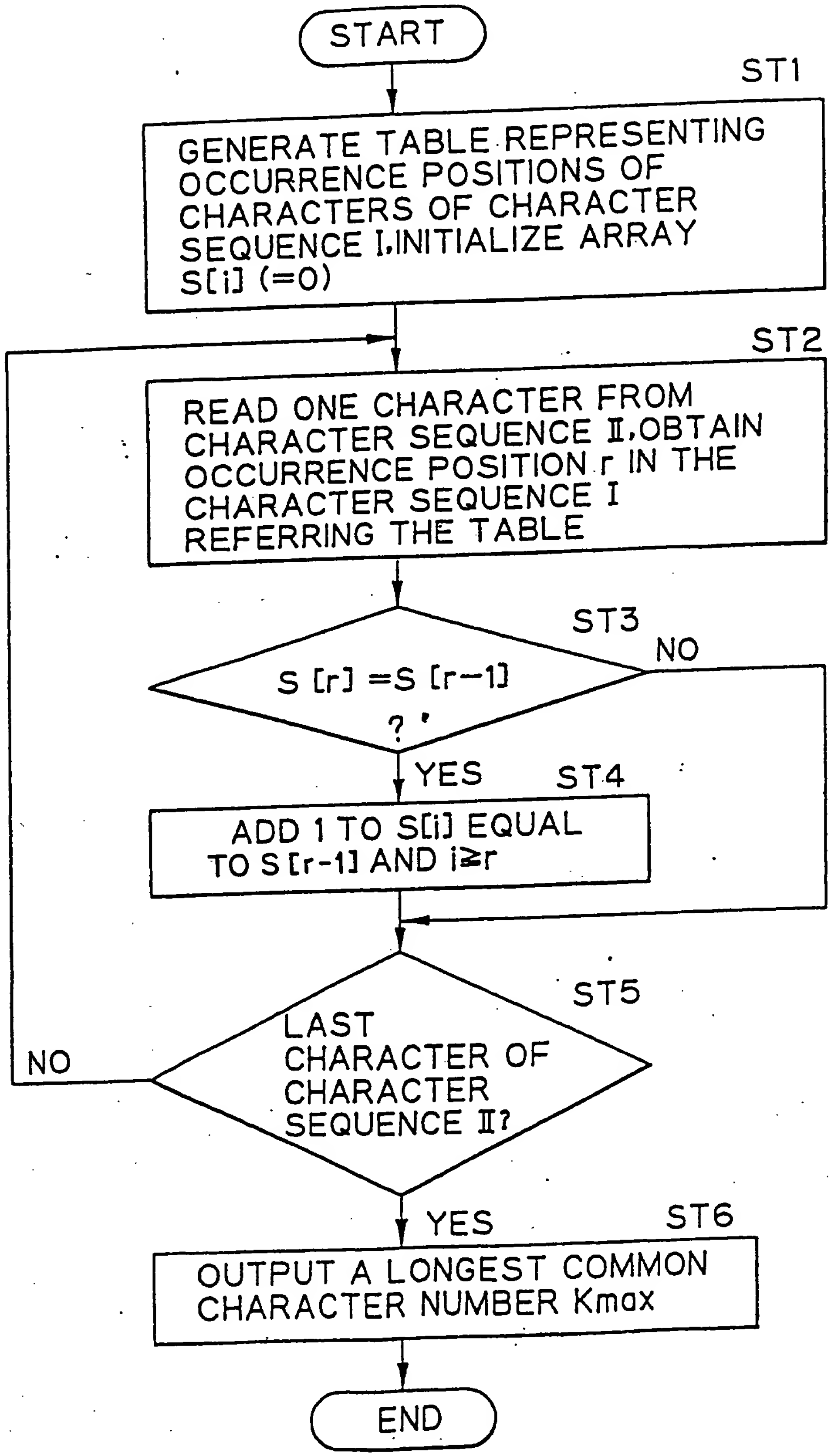

START
ST1
GENERATE TABLE REPRESENTING OCCURRENCE POSITIONS OF CHARACTERS OF CHARACTER SEQUENCE I,INITIALIZE ARRAY S[i] (=0)
ST2
READ ONE CHARACTER FROM CHARACTER SEQUENCE II,OBTAIN OCCURRENCE POSITION r IN THE CHARACTER SEQUENCE I REFERRING THE TABLE
ST3
S [r] =S [r−1] ?
NO
YES
ST4
ADD 1 TO S[i] EQUAL TO S [r−1] AND i≥r
ST5
LAST CHARACTER OF CHARACTER SEQUENCE II?
NO
YES
ST6
OUTPUT A LONGEST COMMON CHARACTER NUMBER Kmax
END

Fig. 3

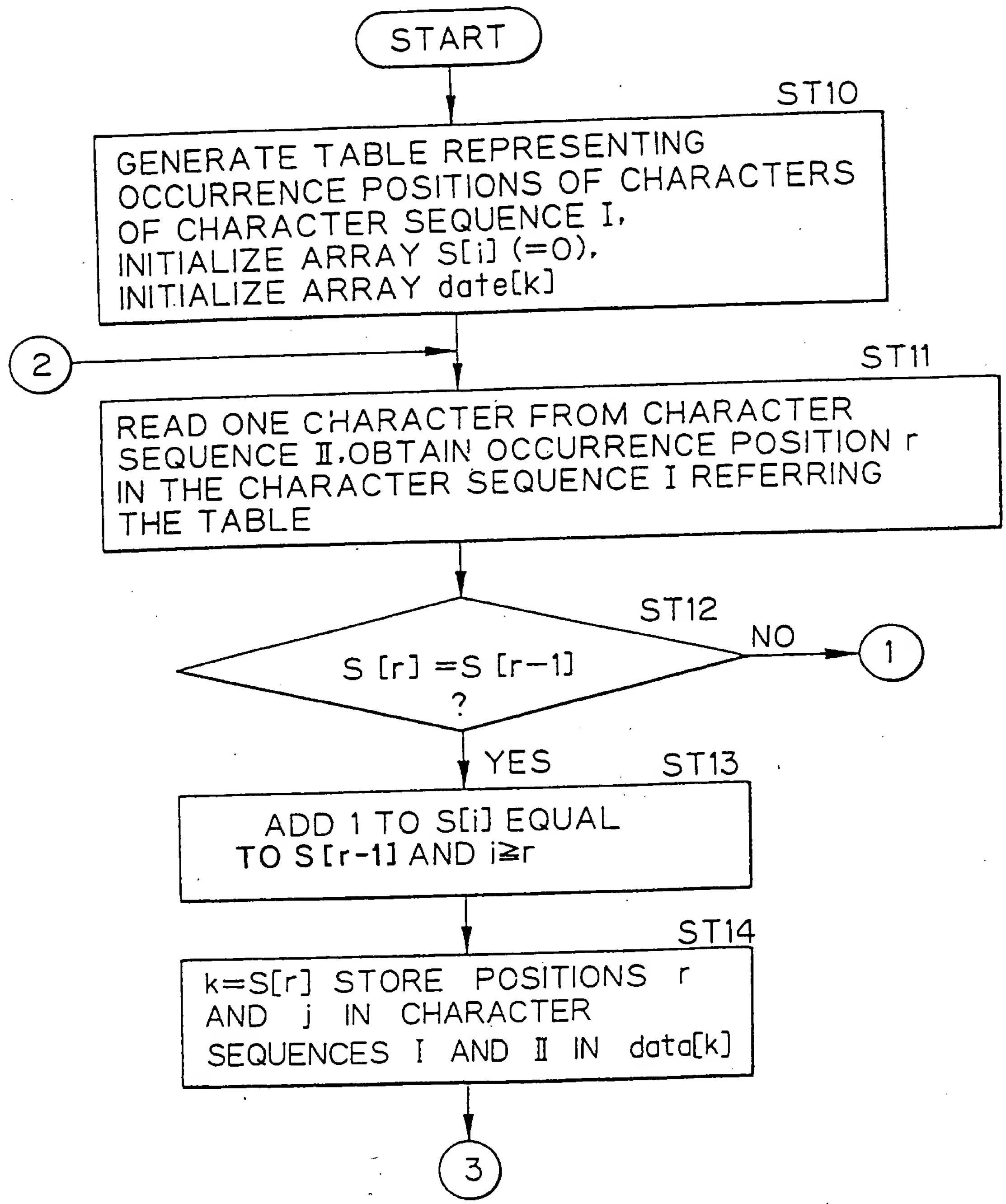

START
ST10
GENERATE TABLE REPRESENTING OCCURRENCE POSITIONS OF CHARACTERS OF CHARACTER SEQUENCE I, INITIALIZE ARRAY S[i] (=0), INITIALIZE ARRAY date[k]
2
ST11
READ ONE CHARACTER FROM CHARACTER SEQUENCE II, OBTAIN OCCURRENCE POSITION r IN THE CHARACTER SEQUENCE I REFERRING THE TABLE
ST12
S [r] =S [r−1] ?
NO
1
YES
ST13
ADD 1 TO S[i] EQUAL TO S[r−1] AND i≥r
ST14
k=S[r] STORE POSITIONS r AND j IN CHARACTER SEQUENCES I AND II IN data[k]
3

Fig. 4

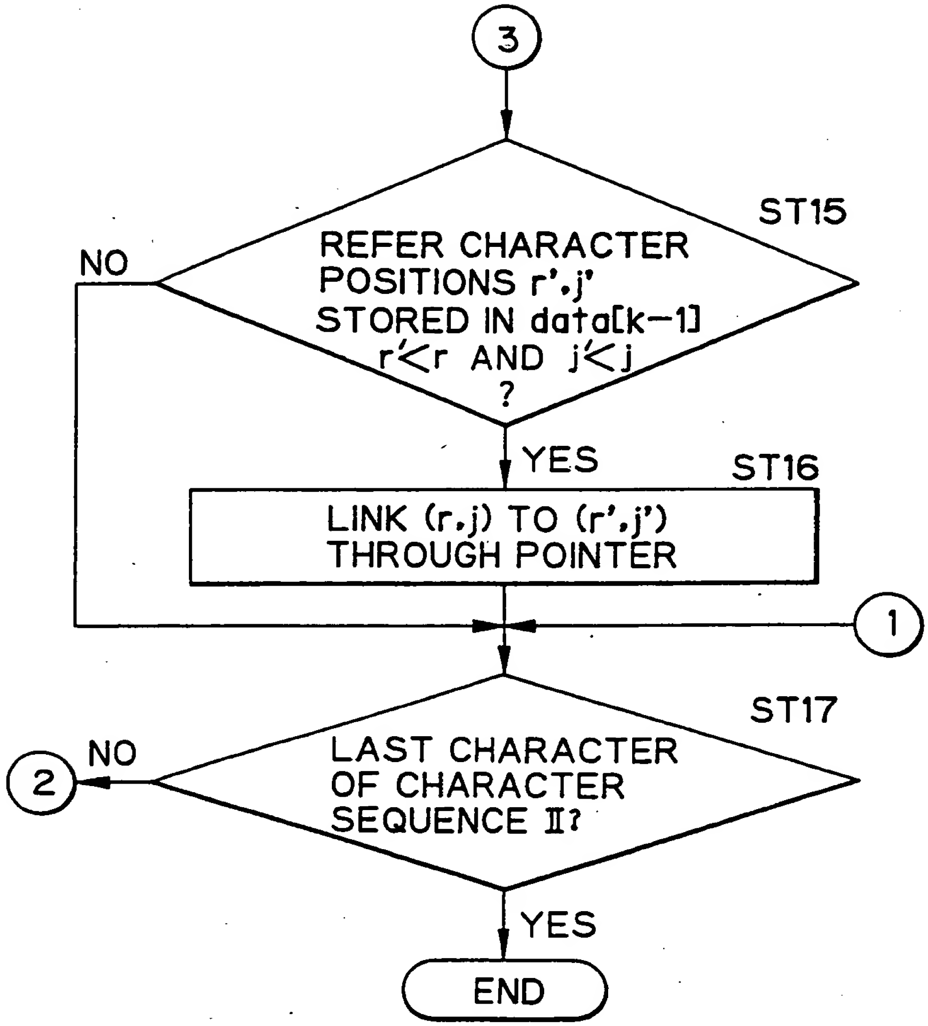

3
REFER CHARACTER POSITIONS r',j' STORED IN data[k-1] r'<r AND j'<j ?
ST15
NO
YES
LINK (r,j) TO (r',j') THROUGH POINTER
ST16
1
LAST CHARACTER OF CHARACTER SEQUENCE II?
ST17
NO
2
YES
END

Fig. 5

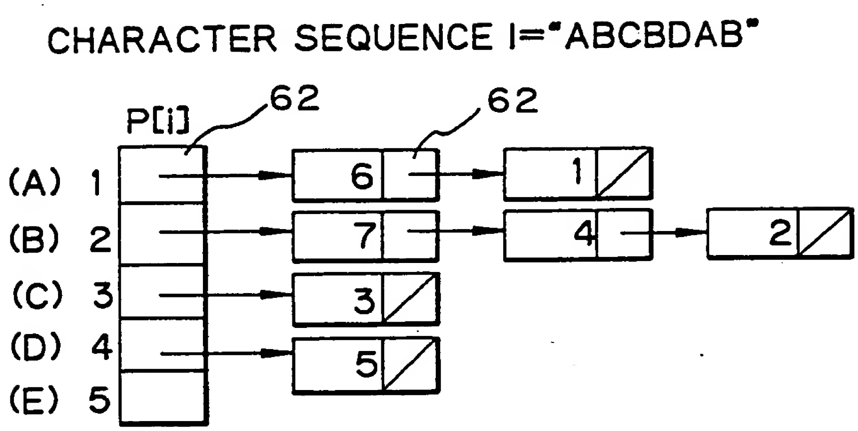
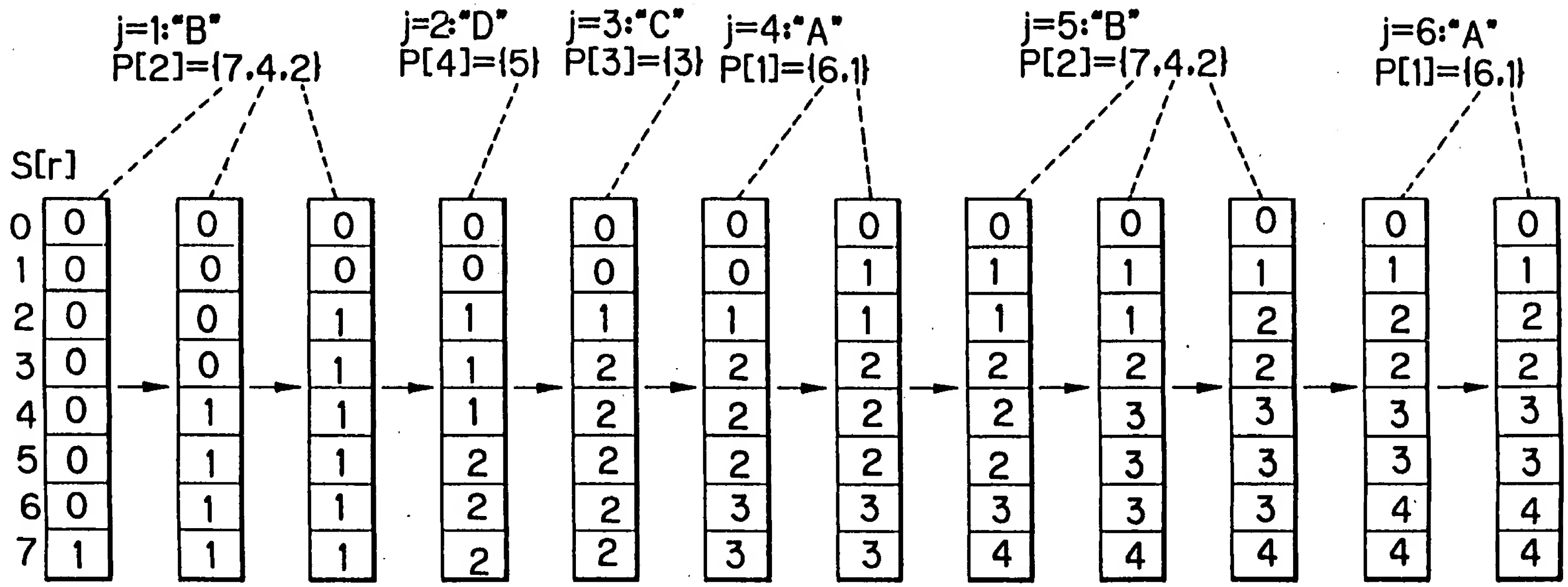


Fig. 6

CHARACTER SEQUENCE II ="BDCABA"



r	S[r]											
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	1	1	1	1	1	1
2	0	0	1	1	1	1	1	1	1	2	2	2
3	0	0	1	1	2	2	2	2	2	2	2	2
4	0	1	1	1	2	2	2	2	3	3	3	3
5	0	1	1	2	2	2	2	2	3	3	3	3
6	0	1	1	2	2	3	3	3	3	3	4	4
7	1	1	1	2	2	3	3	4	4	4	4	4

Fig. 7

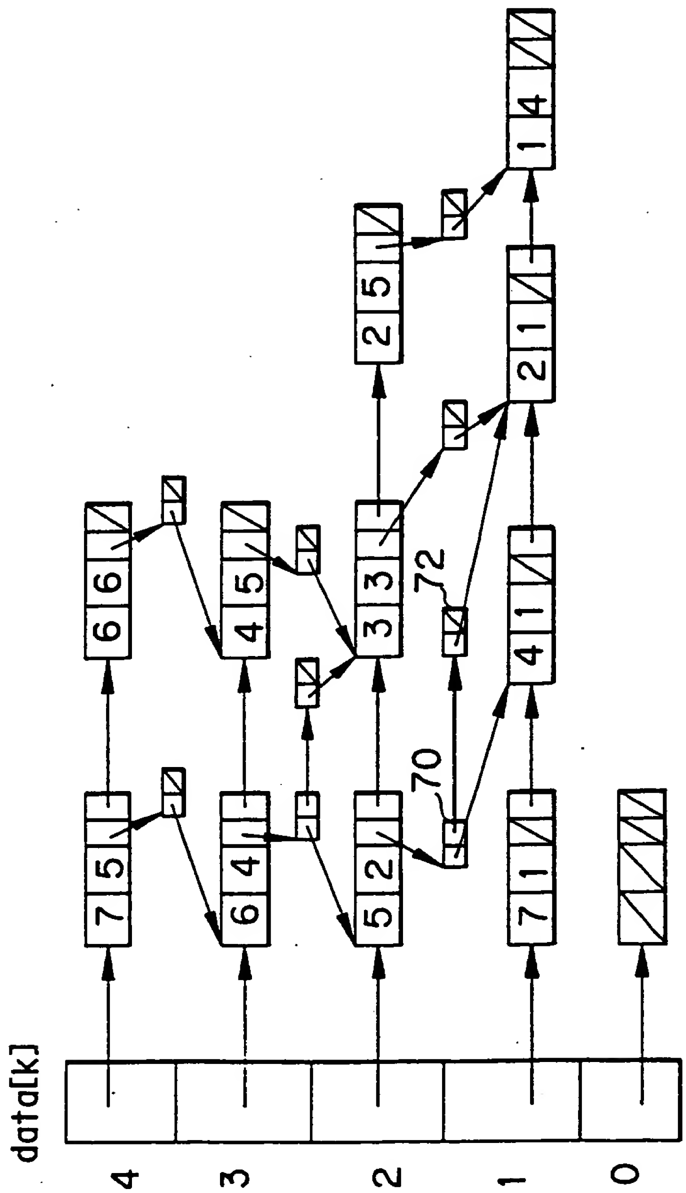
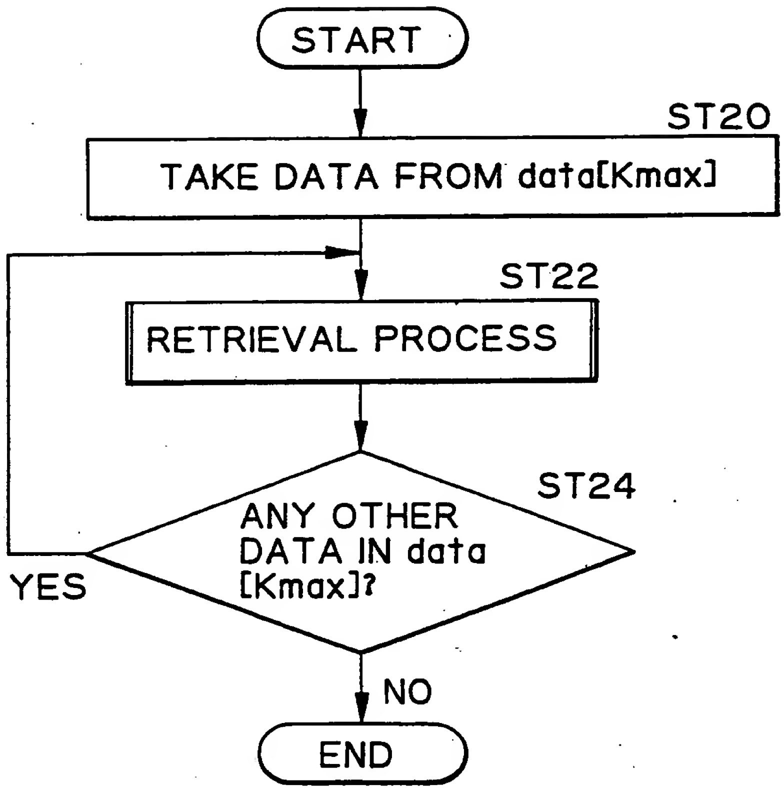


Fig. 8


START
ST20
TAKE DATA FROM data[Kmax]
ST22
RETRIEVAL PROCESS
ST24
ANY OTHER DATA IN data [Kmax]?
YES
NO
END

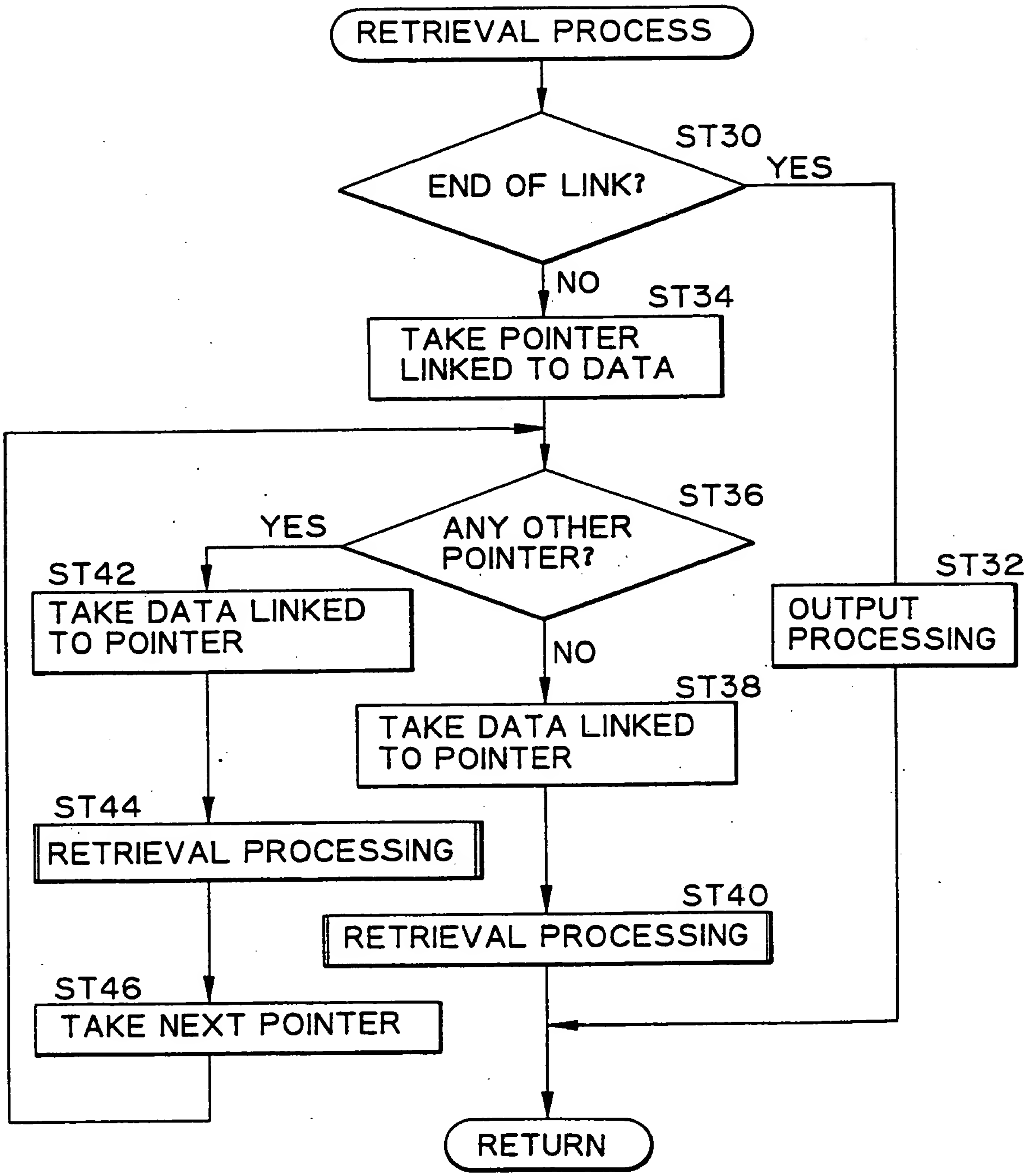

RETRIEVAL PROCESS
ST30
END OF LINK?
YES
NO
ST34
TAKE POINTER LINKED TO DATA
ST36
ANY OTHER POINTER?
YES
ST42
TAKE DATA LINKED TO POINTER
NO
ST38
TAKE DATA LINKED TO POINTER
ST32
OUTPUT PROCESSING
ST44
RETRIEVAL PROCESSING
ST40
RETRIEVAL PROCESSING
ST46
TAKE NEXT POINTER
RETURN

Fig. 9

Fig. 10

human : GDVEKGKKIFIMKCSQCHTVEGGKHKTGPNLHGLFGRK
bacterium : EGDAAAGEKVSKKCLACHTFDQGGANKVGPNPNLFGVF

LCS : GD{x3.3}G{x0.1}K{x0.2}K{x4.0}KC{x2.2}CHT{x3.3}GG{x2.2}K
GD{x1.4}E{x0.2}K{x0.2}K{x0.4}KC{x2.2}CHT{x3.3}GG{x2.2}K

homology : 47%

Fig. 11

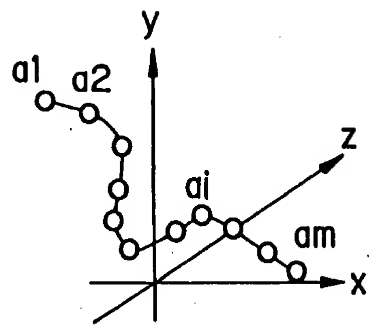
Rat : MSLAILRVIRLVRVFRIFKLSRHSKGLQILGRTLKASMRELGLLIFFIGVV

leucinzip. L{6}L{6}L{6}L{6}L

Fig. 12

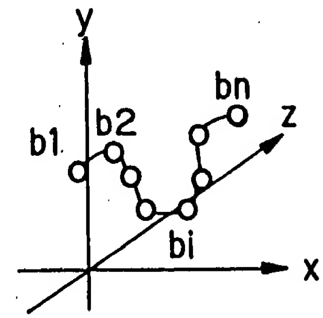
human	: GDVEK G K KIFIMKCSQCHTVEKGG KHKTGPNLHGLFGRK ...
bacterium	: E GDAAAGEKVSK KCLACHTFDQGGANKV GPNPN LFGVF...

Fig. 13 A



A={a1,a2,...ai,...am}

Fig. 13 B



B={b1,b2,...bj,...bn}

Fig. 13C

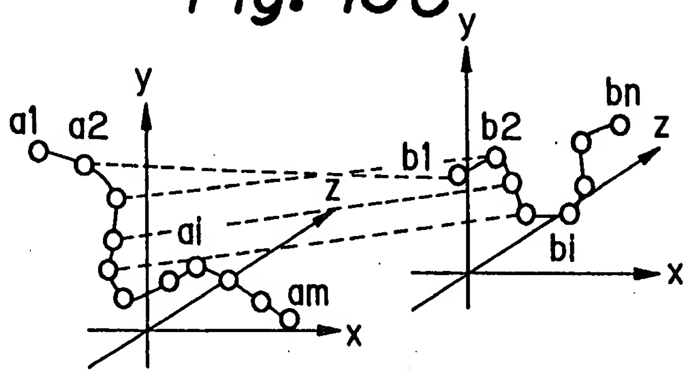


Fig. 13 D

$$r.m.s.d = \frac{\sqrt{\sum_{k=1}^{n} w_k (Ub_k - a_k)^2}}{n}$$

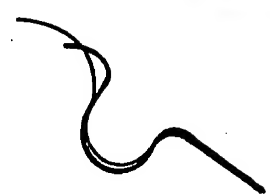


Fig. 15

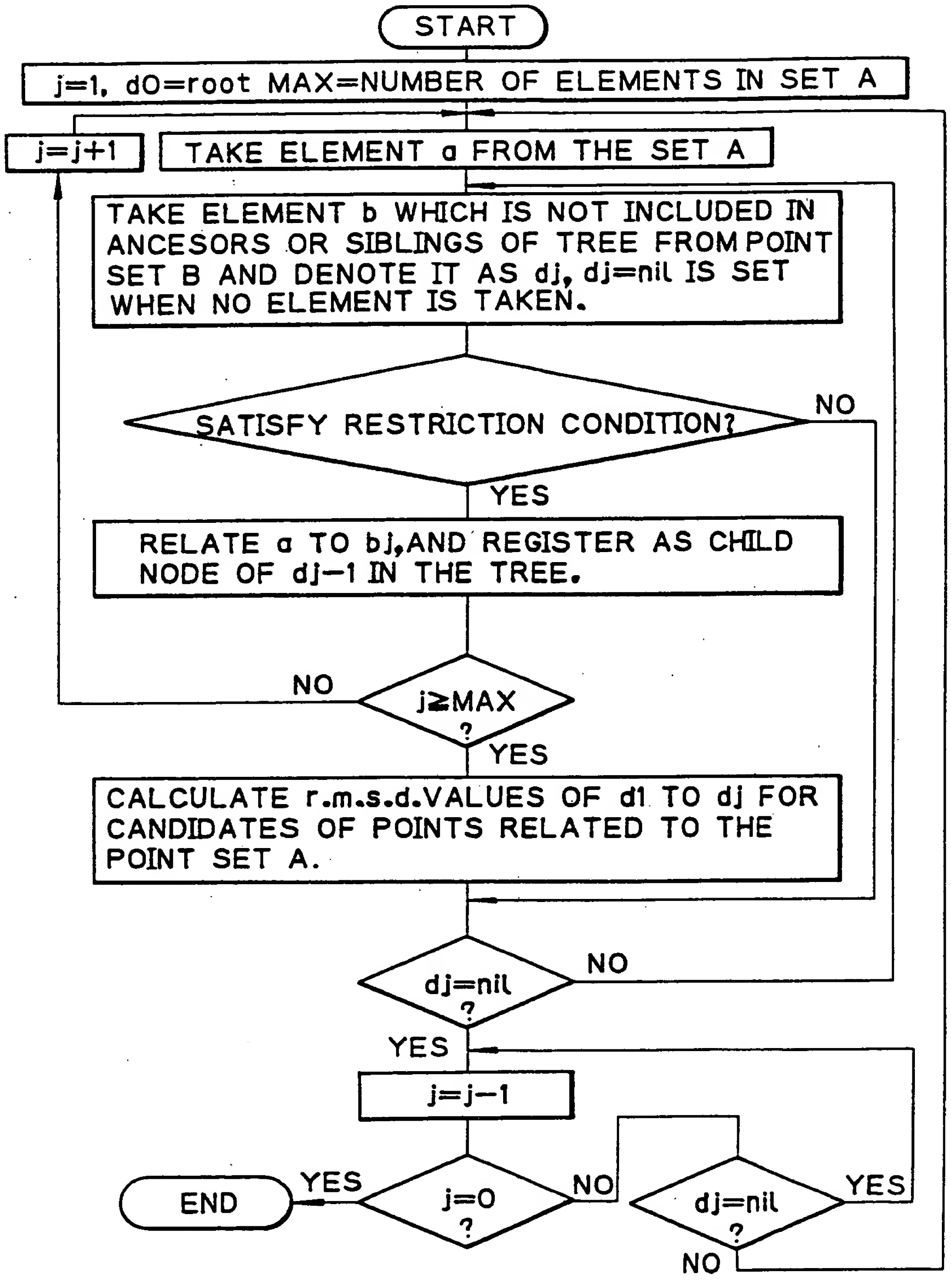

START
j=1, d0=root MAX=NUMBER OF ELEMENTS IN SET A
j=j+1
TAKE ELEMENT a FROM THE SET A
TAKE ELEMENT b WHICH IS NOT INCLUDED IN ANCESORS OR SIBLINGS OF TREE FROM POINT SET B AND DENOTE IT AS dj, dj=nil IS SET WHEN NO ELEMENT IS TAKEN.
SATISFY RESTRICTION CONDITION?
NO
YES
RELATE a TO bj,AND REGISTER AS CHILD NODE OF dj−1 IN THE TREE.
NO
j≧MAX ?
YES
CALCULATE r.m.s.d.VALUES OF d1 TO dj FOR CANDIDATES OF POINTS RELATED TO THE POINT SET A.
dj=nil ?
NO
YES
j=j−1
END
YES
j=0 ?
NO
dj=nil ?
YES
NO

Fig. 14 A

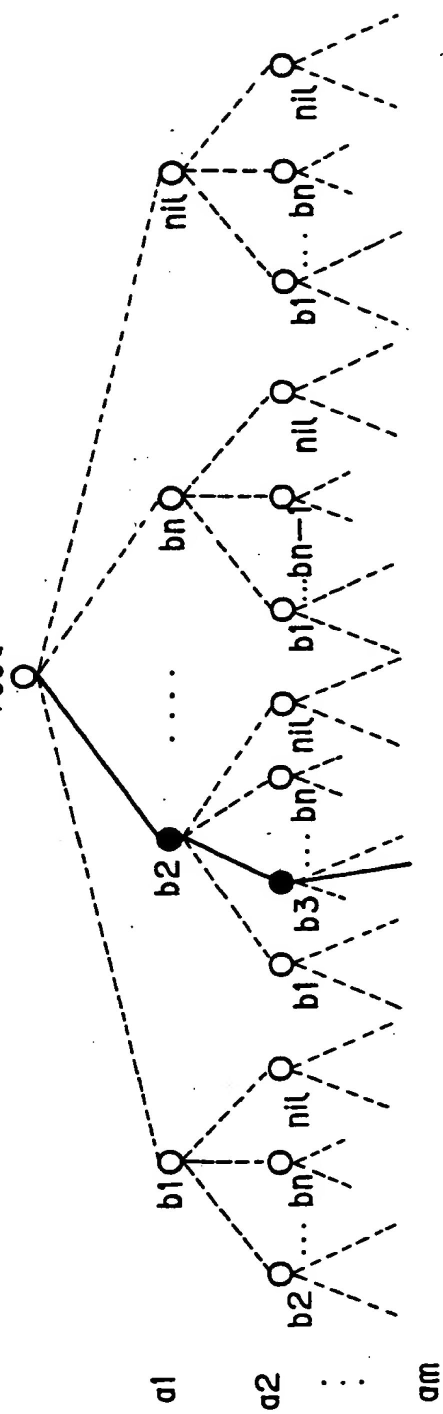


Fig. 14 B

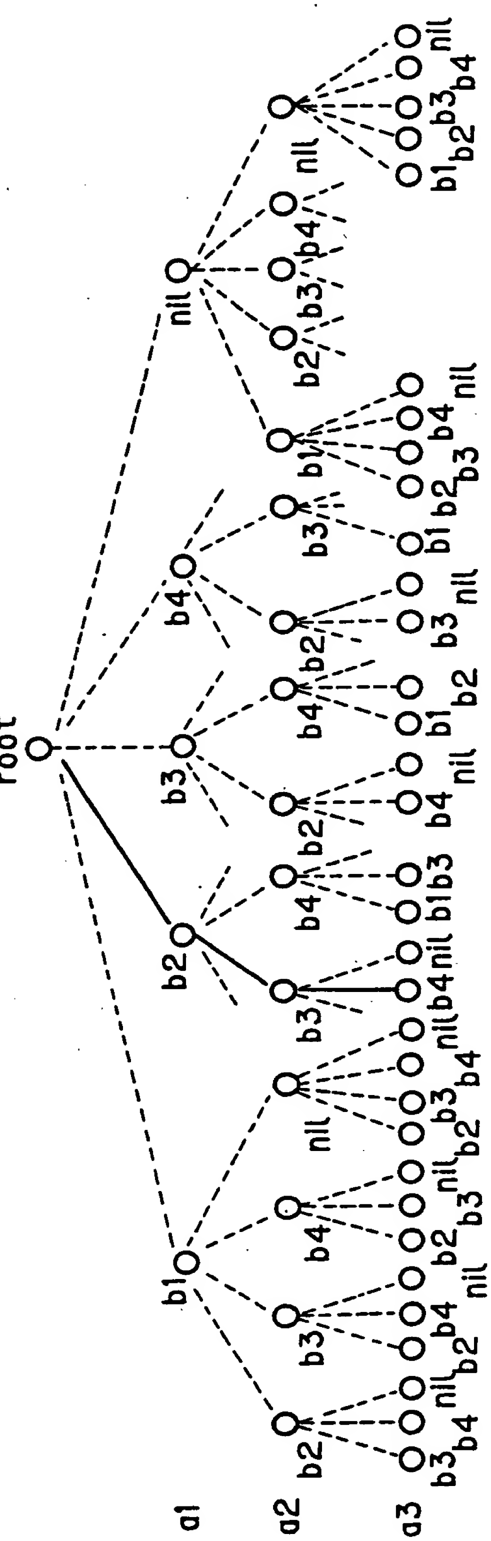


Fig. 16 A

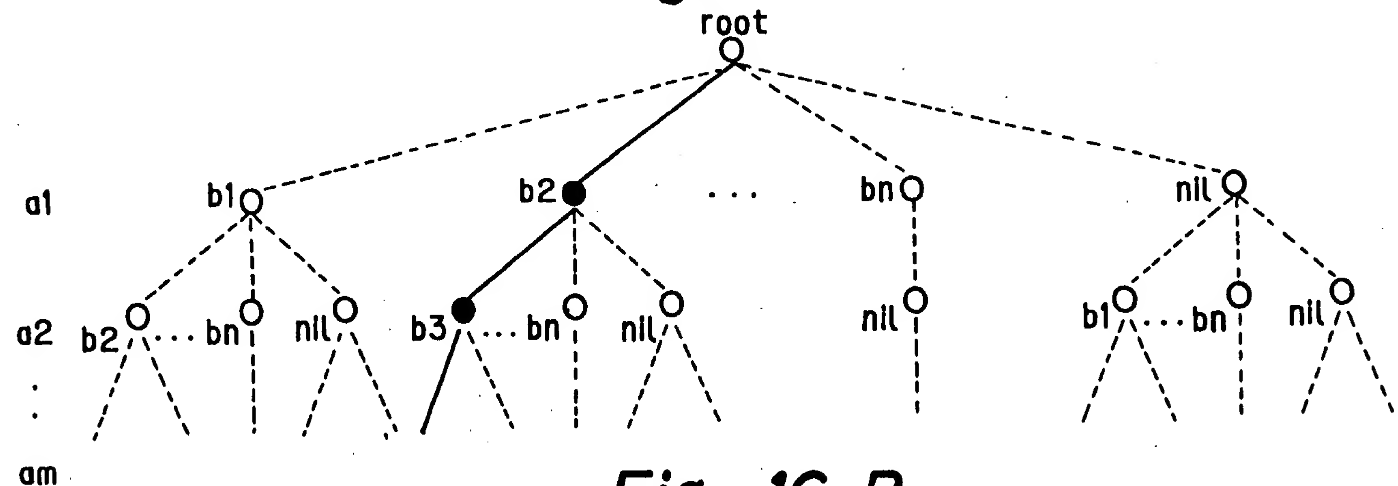


Fig. 16 B

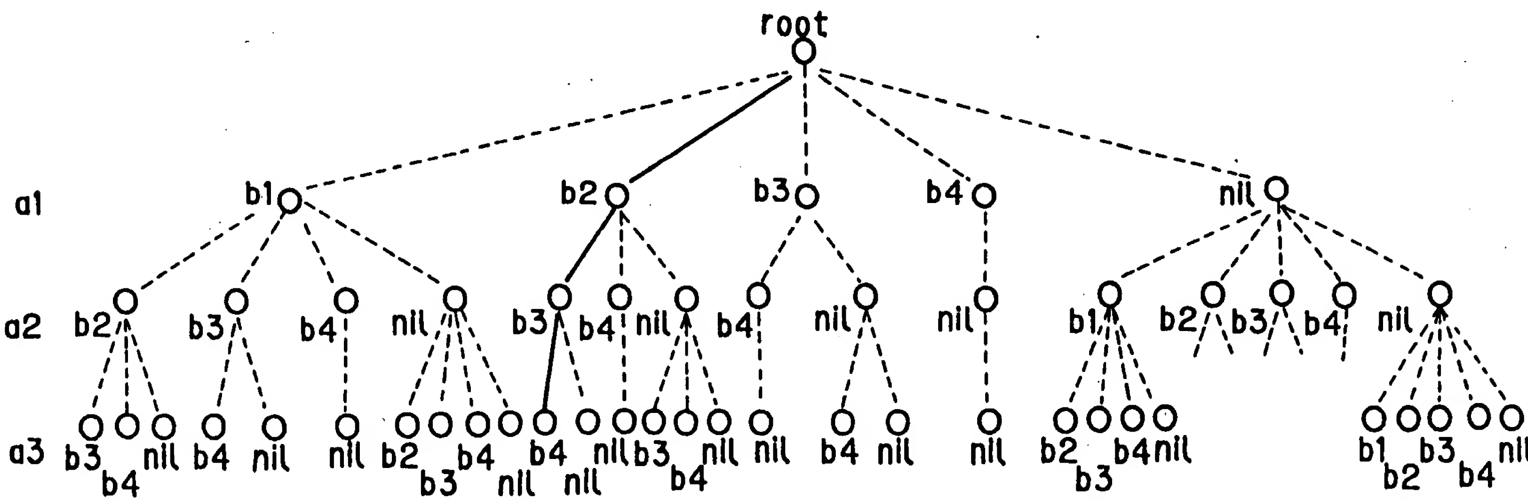


Fig. 17

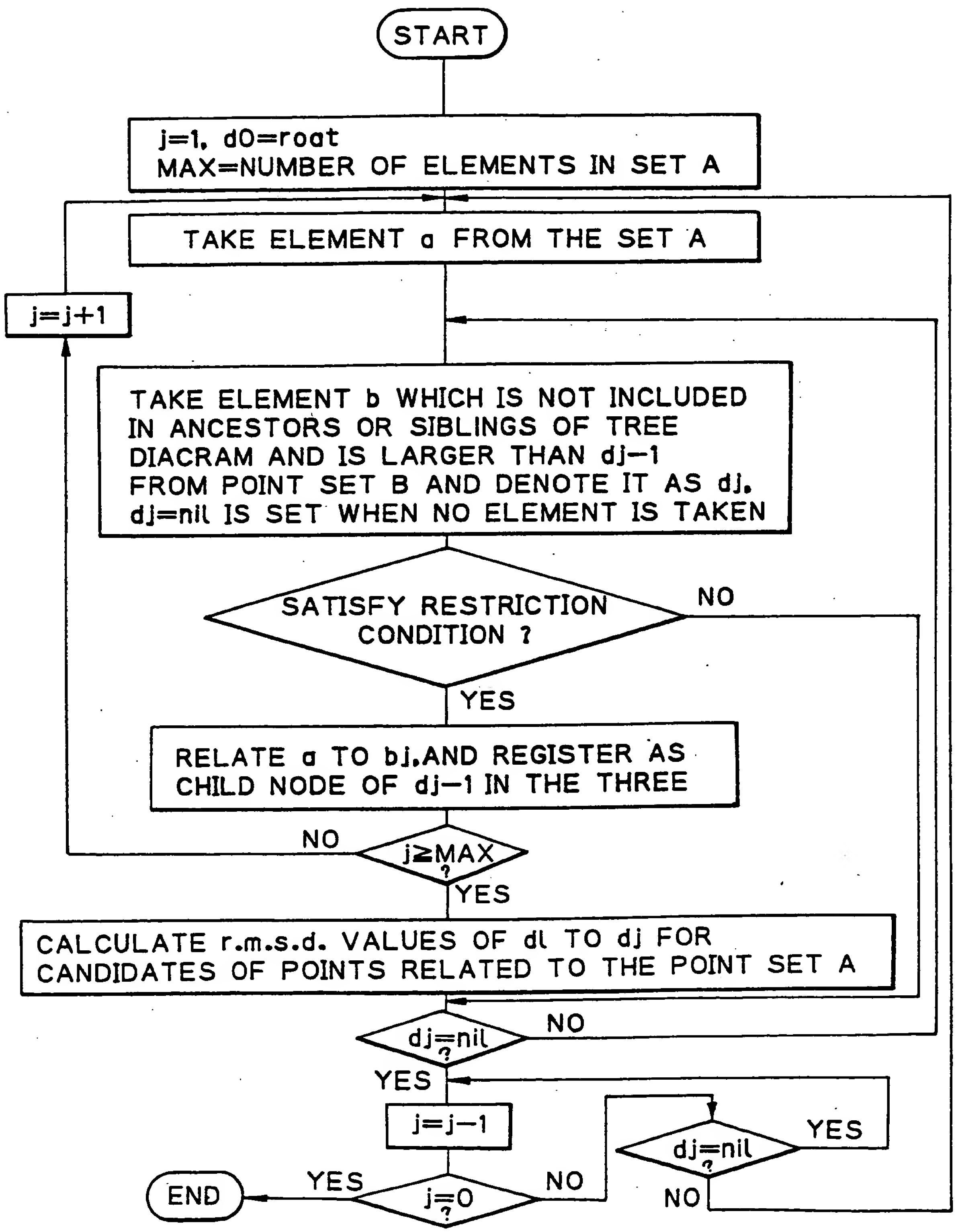

START
j=1, d0=roat
MAX=NUMBER OF ELEMENTS IN SET A
TAKE ELEMENT a FROM THE SET A
j=j+1
TAKE ELEMENT b WHICH IS NOT INCLUDED IN ANCESTORS OR SIBLINGS OF TREE DIACRAM AND IS LARGER THAN dj-1 FROM POINT SET B AND DENOTE IT AS dj. dj=nil IS SET WHEN NO ELEMENT IS TAKEN
SATISFY RESTRICTION CONDITION ?
NO
YES
RELATE a TO bj.AND REGISTER AS CHILD NODE OF dj-1 IN THE THREE
NO
j≥MAX ?
YES
CALCULATE r.m.s.d. VALUES OF dl TO dj FOR CANDIDATES OF POINTS RELATED TO THE POINT SET A
dj=nil ?
NO
YES
j=j-1
dj=nil ?
YES
NO
END
YES
j=0 ?
NO

Fig. 18

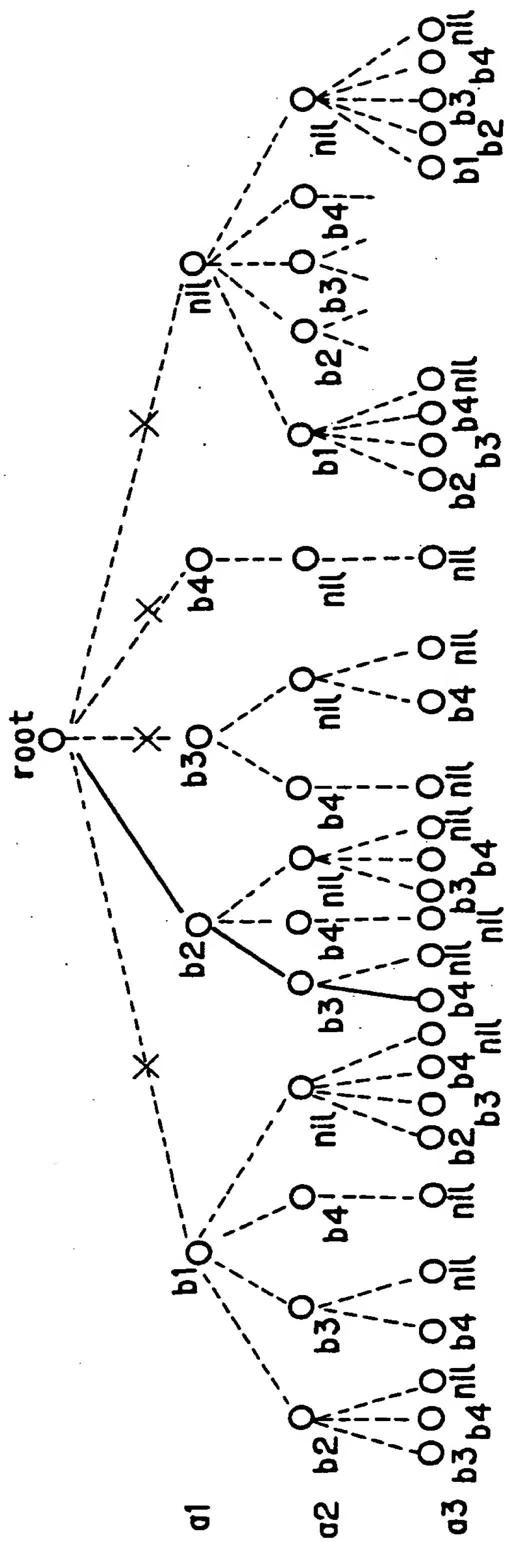


Fig. 19 A

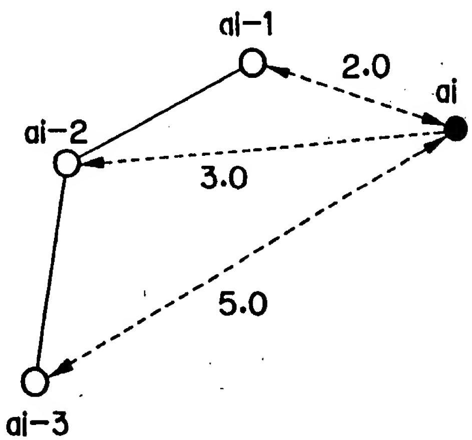


Fig. 19 B

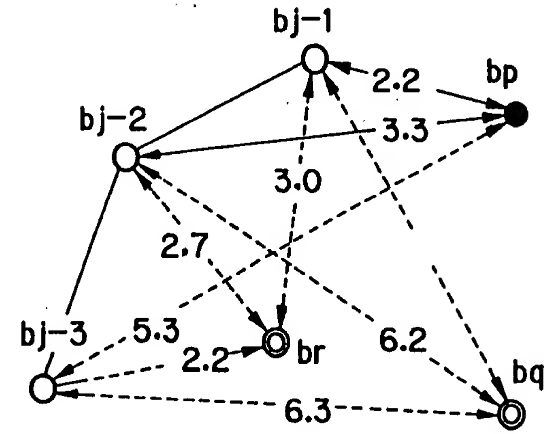


Fig. 20 A

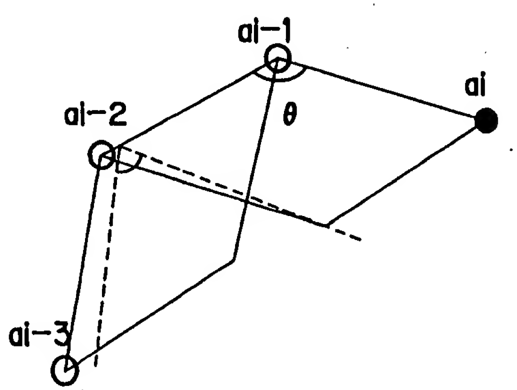


Fig. 20 B

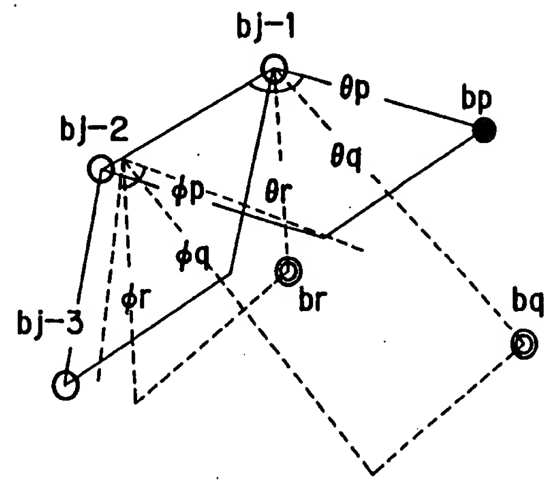


Fig. 21

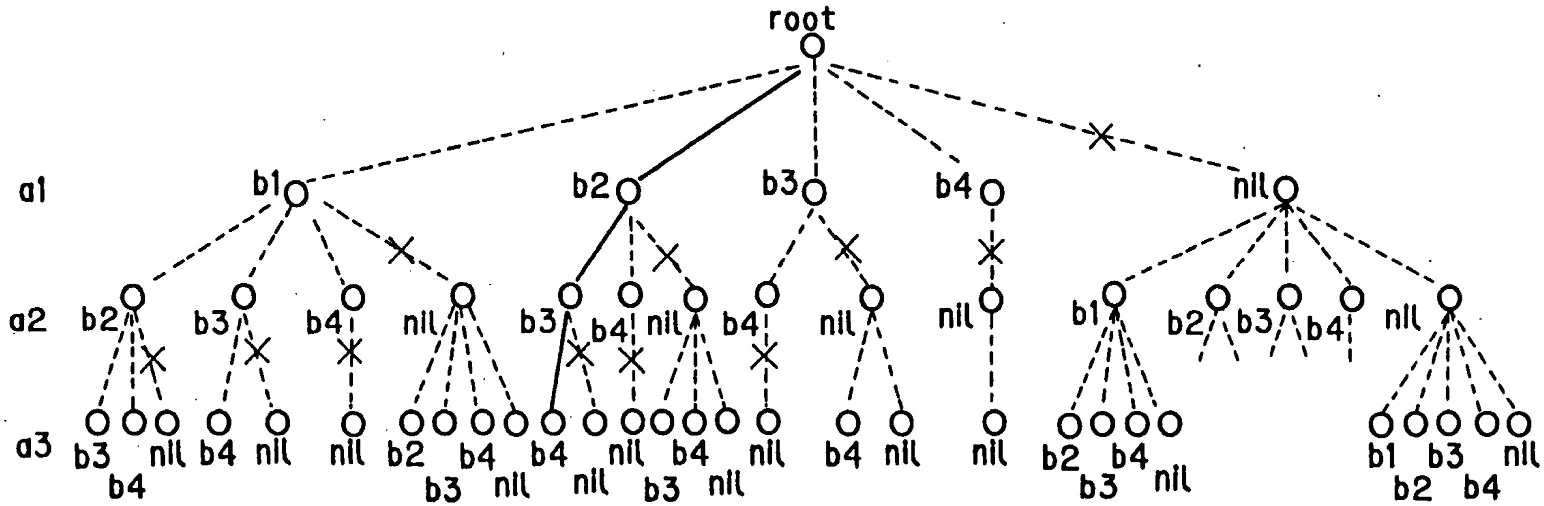


Fig. 22

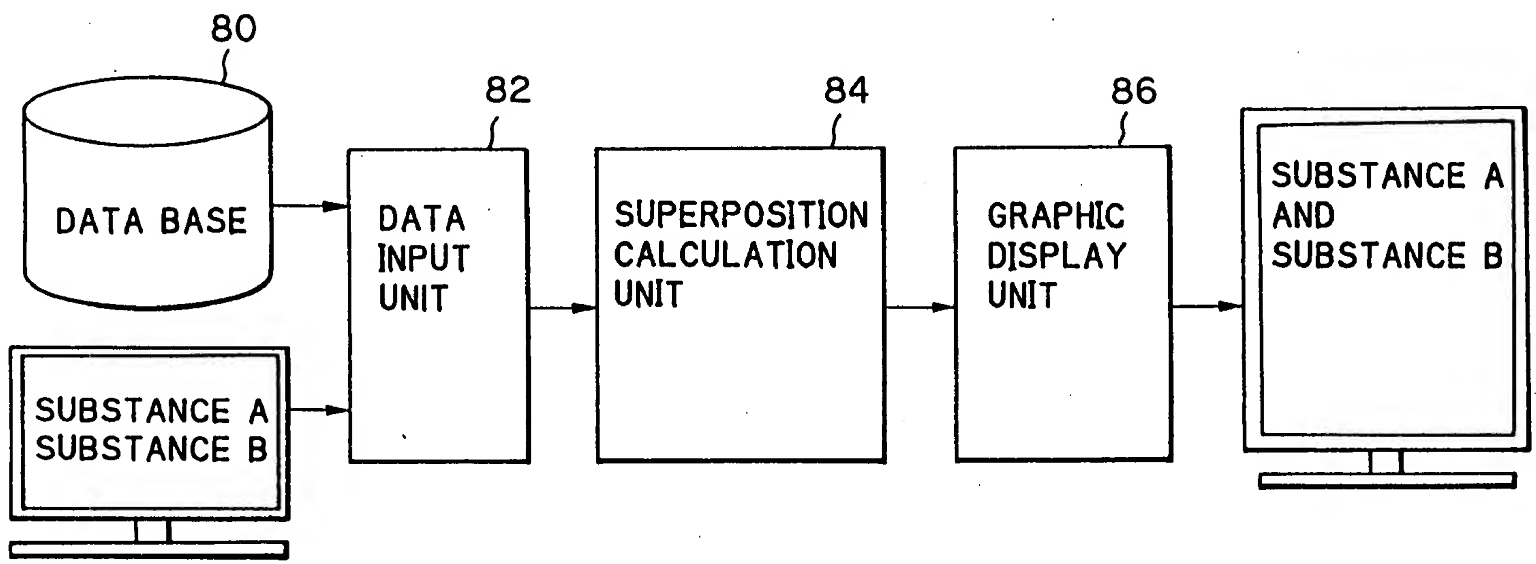

80
DATA BASE
SUBSTANCE A
SUBSTANCE B
82
DATA INPUT UNIT
84
SUPERPOSITION CALCULATION UNIT
86
GRAPHIC DISPLAY UNIT
SUBSTANCE A AND SUBSTANCE B

Fig. 23 A

1	T E E Q I A E F K E	A F S L F D K D G D
21	G T I T T K E L G T	V M R S L G Q N P T
41	E A E L Q D M I N E	V D A D G N G T I D
61	F P E F L T M M A R	K M K D T D S E E E
81	I R E A F R V F D K	D G N G Y I S A A E
101	L R H V M T N L G E	K L T D E E V D E M
121	I R E A N I D G D G	Q V N Y E E F V Q M
141	M T A	

AMINO ACID SEQUENCE OF CALMODULIN
(EXCERPT FROM PDB)

Fig. 23 B

1	A M D Q Q A E A R A	F L S E E M I A E F
21	K A A F D M F D A D	G G G D I S T K E L
41	G T V M R M L G Q N	P T K E E L D A I I
61	E E V D E D G S G T	I D F E E F L V M
81	V R Q M K E D A K G	K S E E E L A D C F
101	R I F D K N A D G F	I D I E E L G E I L
121	R A T G E H V T E E	D I E D L M K D S D
141	K N N D G R I D F D	E F L K M M E G V Q
161		

AMINO ACID SEQUENCE OF TROPONIN C
(EXCERPT FROM PDB)

Fig. 24 A

CALMODULIN

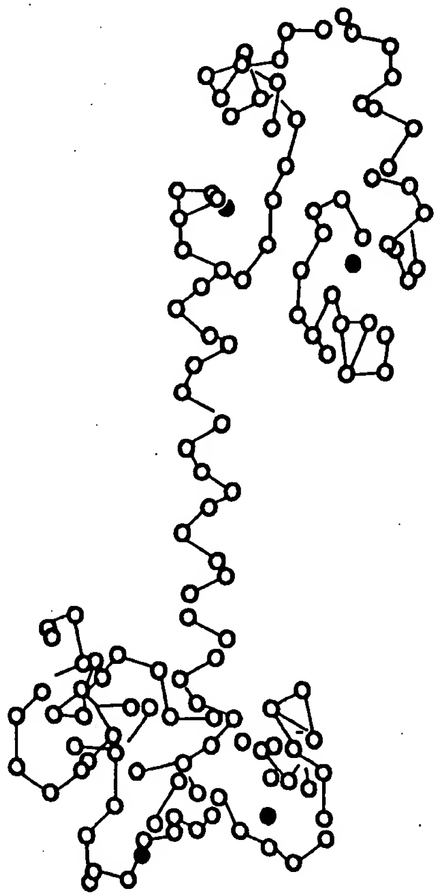


Fig. 24 B

TROPONIN C

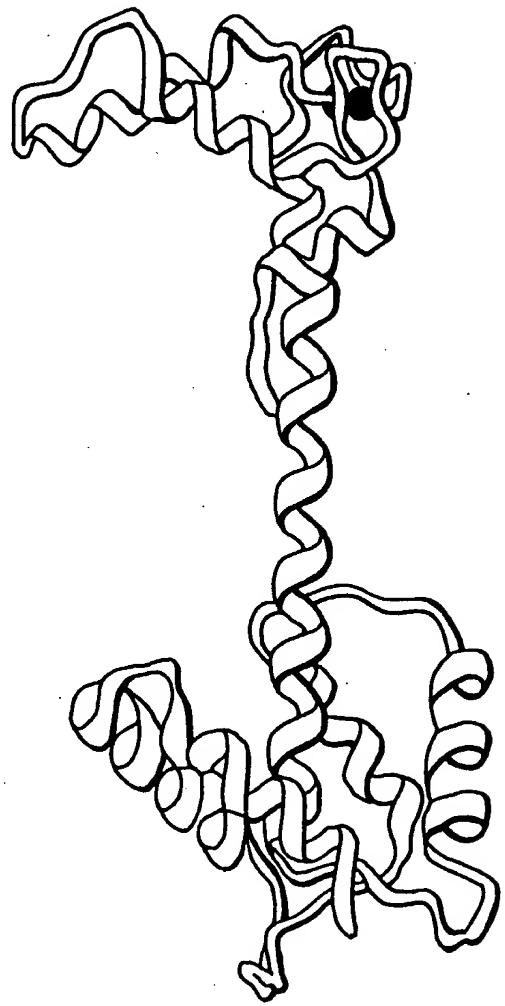


Fig. 25

Probe site = 81-108 in Calmodulin

96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	
L	A	D	C	F	R	I	F	D	K	N	A	D	G	F	< target >
I	R	E	A	F	R	V	F	D	K	D	G	N	G	Y	< probe >
111	112	113	114	115	116	117	118	119	120	121	122	123			
I	D	I	E	E	L	G	E	I	L	R	A	T	< target >		
I	S	A	A	E	L	R	H	V	M	T	N	L	< probe >		

rmsd = 0.567034

Fig. 26

Probe site = 81-108 and 117-143 in Calmodulin

96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	
L	A	D	C	F	R	I	F	D	K	N	A	D	G	F	< target >
I	R	E	A	F	R	V	F	D	K	D	G	N	G	Y	< probe >
111	112	113	114	115	116	117	118	119	120	121	122	123			
I	D	I	E	E	L	G	E	I	L	R	A	T	< target >		
I	S	A	A	E	L	R	H	V	M	T	N	L	< probe >		
132	133	134	135	136	137	138	139	140	141	142	143	144	145		
I	E	D	L	M	K	D	S	D	K	N	N	D	G	< target >	
V	D	E	M	I	R	E	A	N	I	D	G	D	G	< probe >	
146	147	148	149	150	151	152	153	154	155	156	157	158			
R	I	D	F	D	E	F	L	K	M	M	E	G	< target >		
Q	V	N	Y	E	E	F	V	Q	M	M	T	A	< probe >		

rmsd = 0.823665

Fig. 27

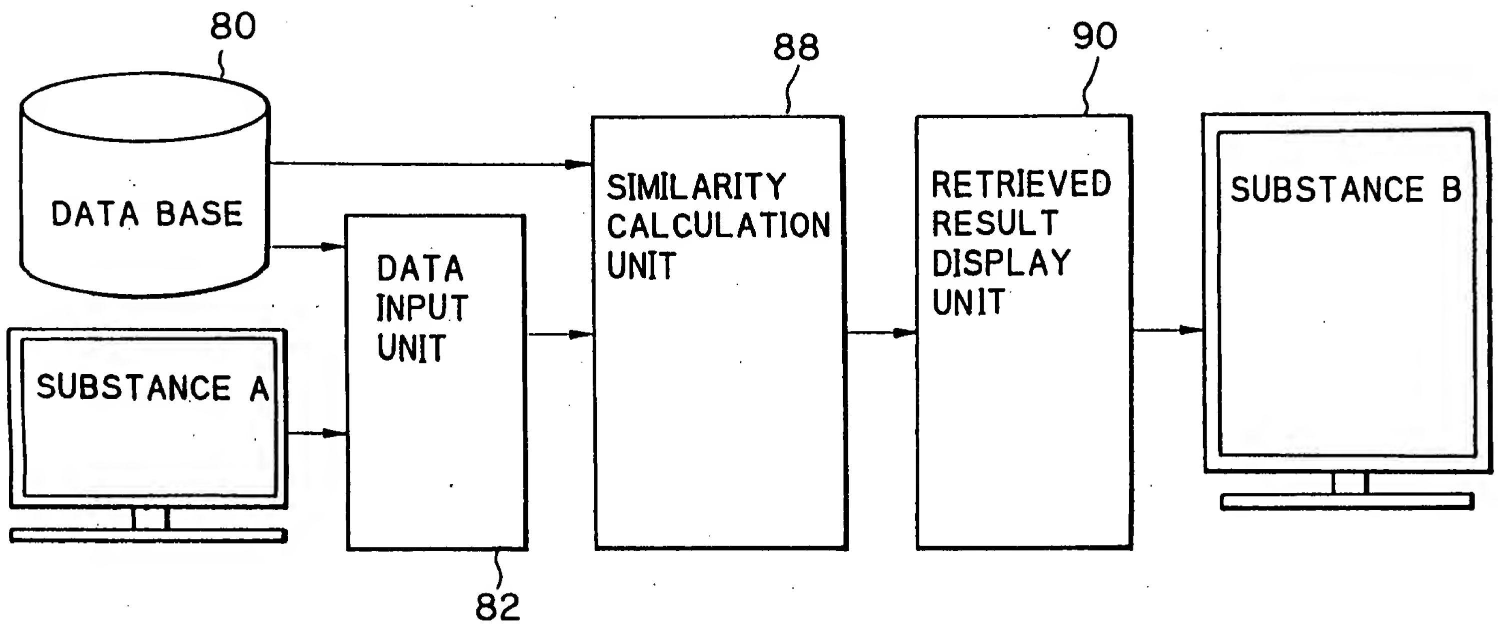

80
DATA BASE
SUBSTANCE A
DATA INPUT UNIT
82
88
SIMILARITY CALCULATION UNIT
90
RETRIEVED RESULT DISPLAY UNIT
SUBSTANCE B

Fig. 28

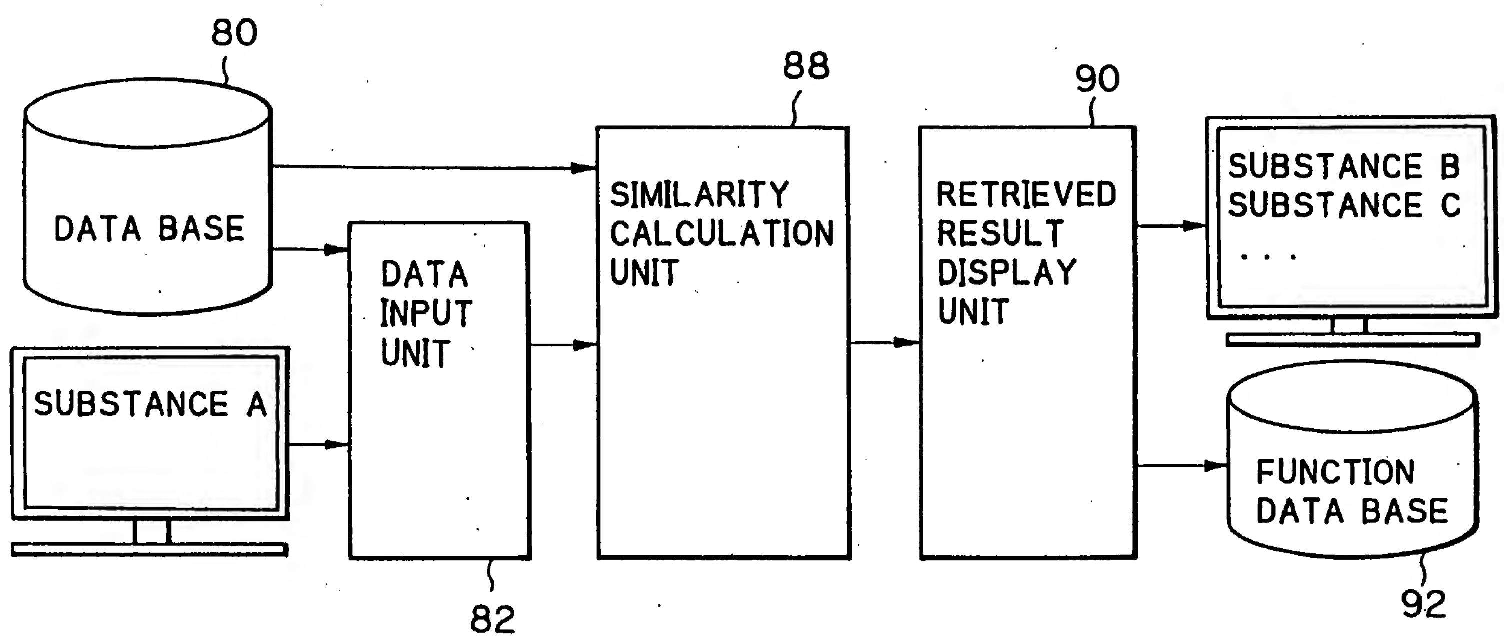

80
DATA BASE
SUBSTANCE A
DATA
INPUT
UNIT
82
88
SIMILARITY
CALCULATION
UNIT
90
RETRIEVED
RESULT
DISPLAY
UNIT
SUBSTANCE B
SUBSTANCE C
. . .
FUNCTION
DATA BASE
92

Fig. 29

```
=================== ATP/GTP binding site ==========================

Probe = (elongation factor)

7 8 9 10 11 12 13 14
G H V  D  H  G  K  T  < probe  >

-----
8 9 10 11 12 13 14 15
G A p  G  S  G  K  G  < target >
G H V  D  H  G  K  T  < probe  >
rmsd=0.648732   adenylate kinase

unit - A

      .         .         .
      .         .         .
      .         .         .

10 11 12 13 14 15 16 17
 G  A  G  G  V  G  K  S  < target >
 G  H  V  D  H  G  K  T  < probe  >
rmsd=0.421770   ras protein
```

Fig. 30

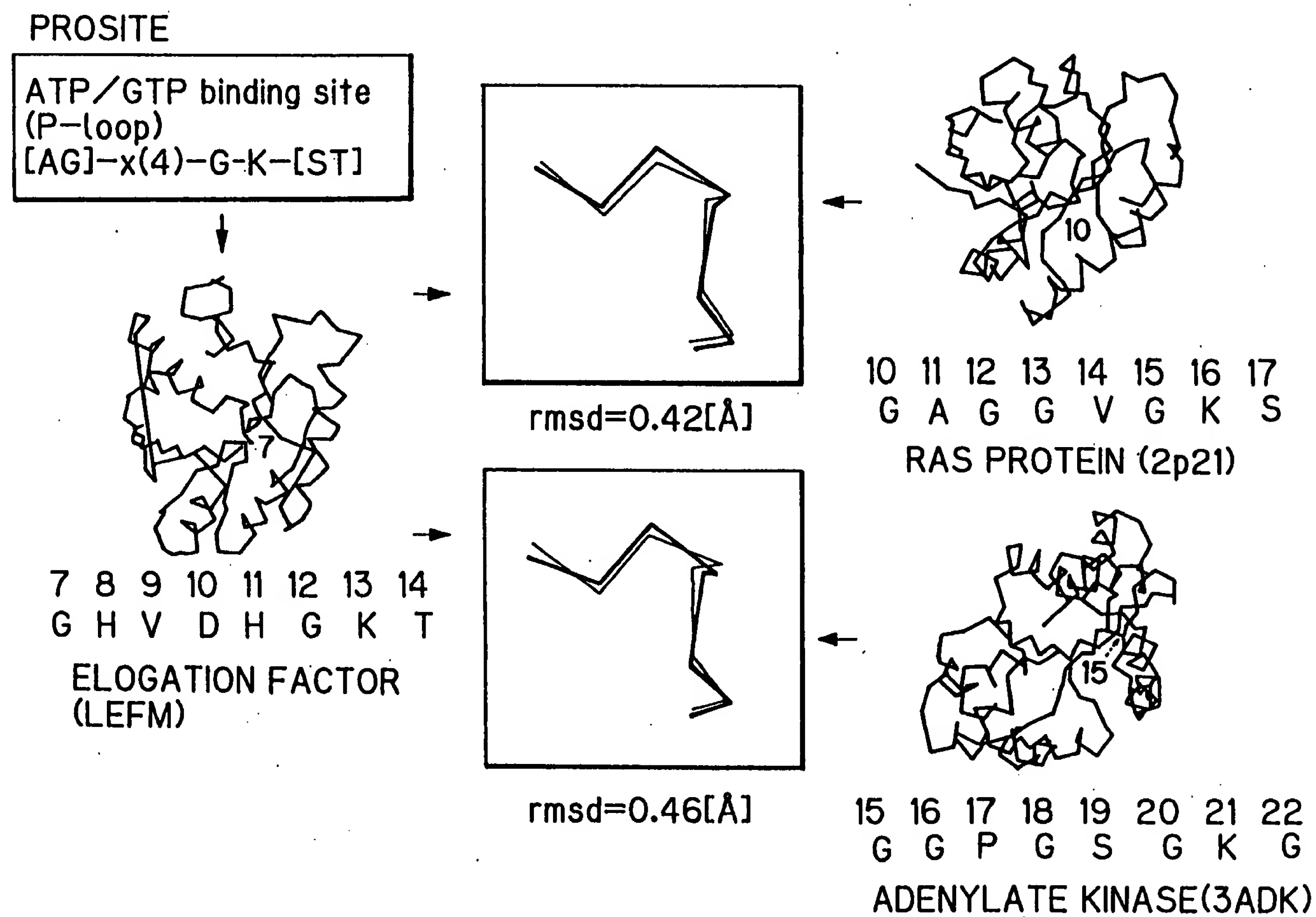

PROSITE
ATP/GTP binding site
(P-loop)
[AG]-x(4)-G-K-[ST]
10
7
rmsd=0.42[Å]
rmsd=0.46[Å]
15
10 11 12 13 14 15 16 17
G A G G V G K S
RAS PROTEIN (2p21)
7 8 9 10 11 12 13 14
G H V D H G K T
ELOGATION FACTOR
(LEFM)
15 16 17 18 19 20 21 22
G G P G S G K G
ADENYLATE KINASE(3ADK)

Fig. 31

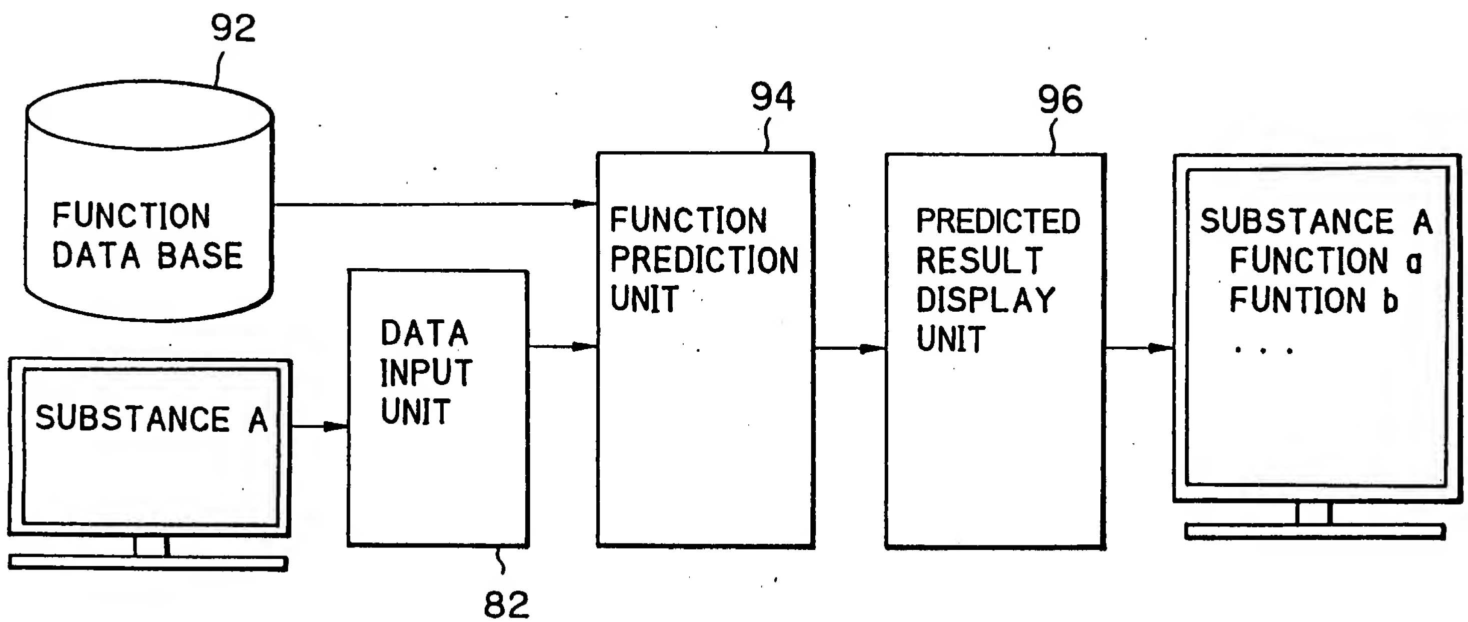

92
FUNCTION DATA BASE
SUBSTANCE A
DATA INPUT UNIT
82
94
FUNCTION PREDICTION UNIT
96
PREDICTED RESULT DISPLAY UNIT
SUBSTANCE A
FUNCTION a
FUNTION b
. . .

Fig. 32 A

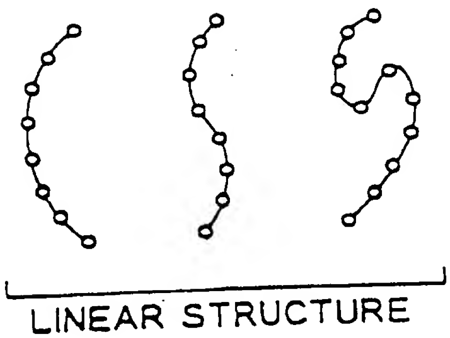


Fig. 32 B

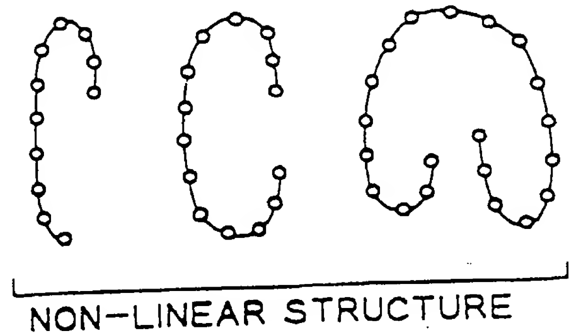


Fig. 33

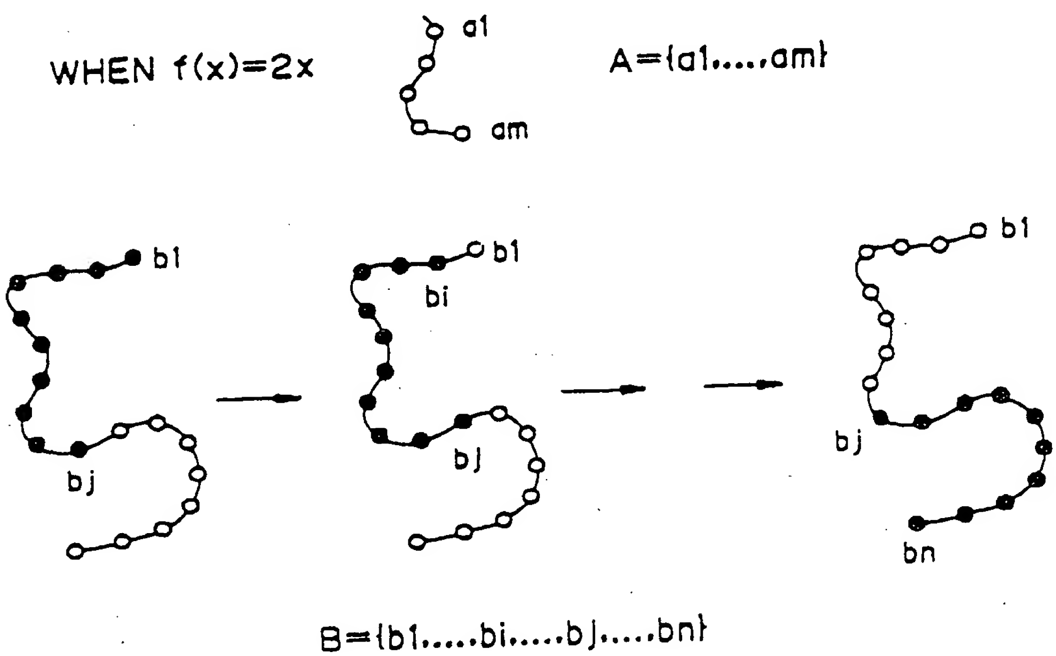


Fig. 34

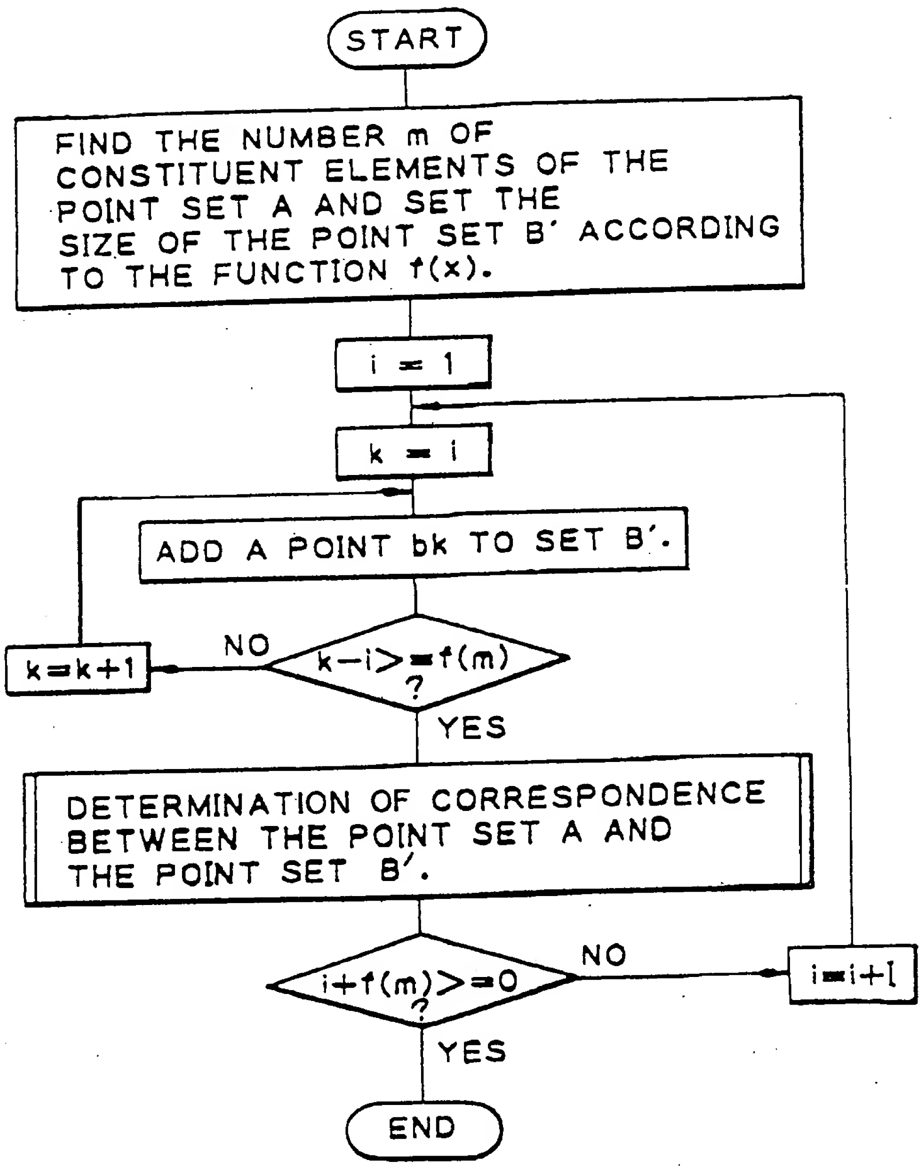
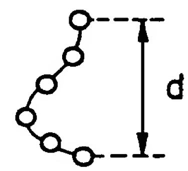
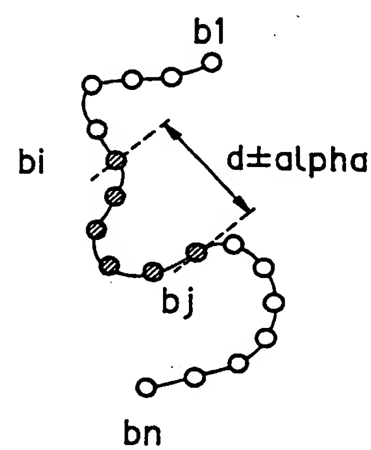

START
FIND THE NUMBER m OF CONSTITUENT ELEMENTS OF THE POINT SET A AND SET THE SIZE OF THE POINT SET B' ACCORDING TO THE FUNCTION f(x).
i = 1
k = i
ADD A POINT bk TO SET B'.
k−i>=f(m) ?
NO
k=k+1
YES
DETERMINATION OF CORRESPONDENCE BETWEEN THE POINT SET A AND THE POINT SET B'.
i+f(m)>=0 ?
NO
i=i+1
YES
END

Fig. 35 A



A={a1,a2,....,am}

Fig. 35 B



B={b1,....,bi,....,bj,....,bn}

Fig. 36

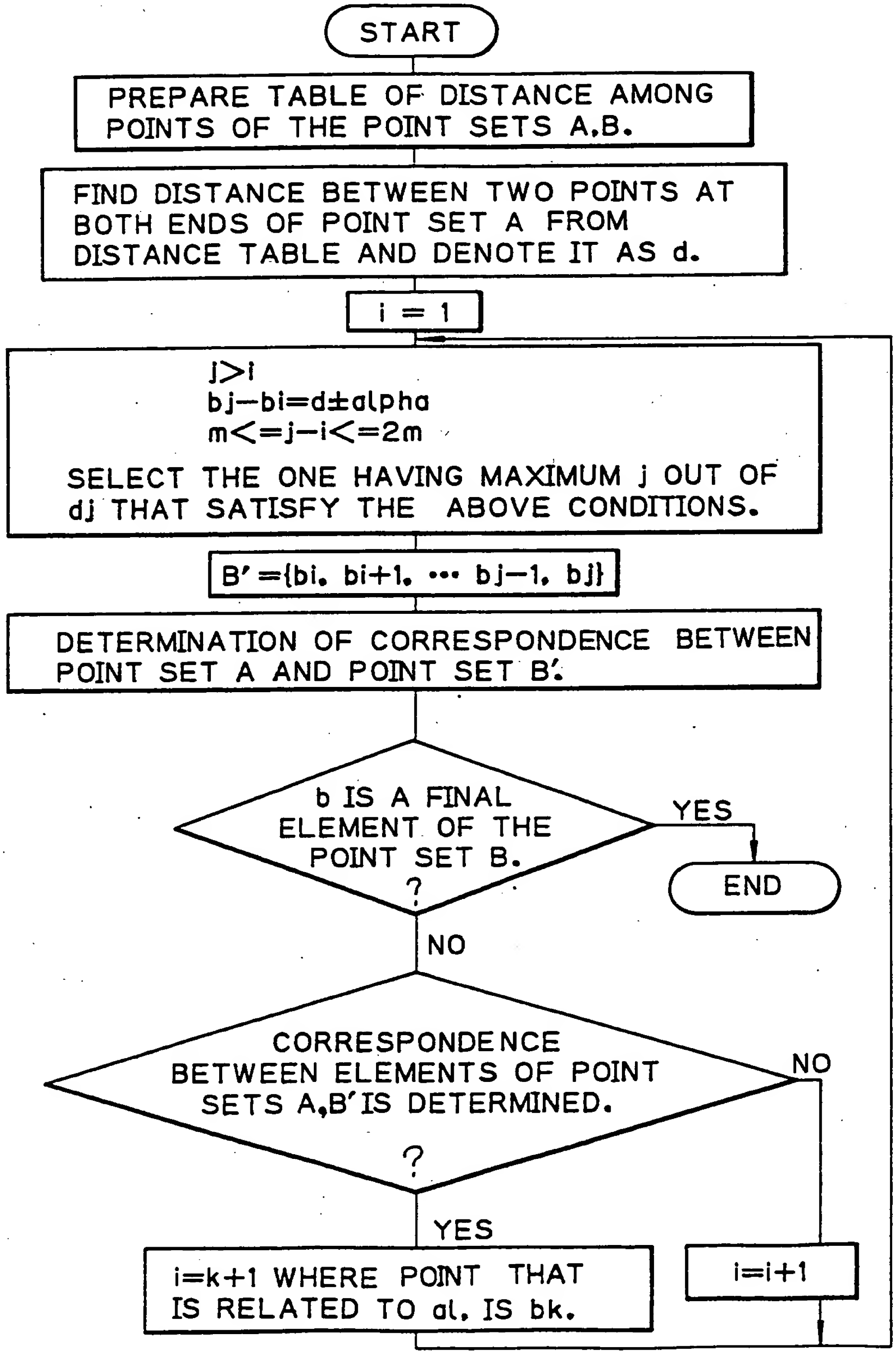

START
PREPARE TABLE OF DISTANCE AMONG POINTS OF THE POINT SETS A,B.
FIND DISTANCE BETWEEN TWO POINTS AT BOTH ENDS OF POINT SET A FROM DISTANCE TABLE AND DENOTE IT AS d.
i = 1
j>i
bj−bi=d±alpha
m<=j−i<=2m
SELECT THE ONE HAVING MAXIMUM j OUT OF dj THAT SATISFY THE ABOVE CONDITIONS.
B′={bi, bi+1, ••• bj−1, bj}
DETERMINATION OF CORRESPONDENCE BETWEEN POINT SET A AND POINT SET B′.
b IS A FINAL ELEMENT OF THE POINT SET B. ?
YES
END
NO
CORRESPONDENCE BETWEEN ELEMENTS OF POINT SETS A,B′ IS DETERMINED. ?
NO
YES
i=k+1 WHERE POINT THAT IS RELATED TO al, IS bk.
i=i+1

Fig. 37

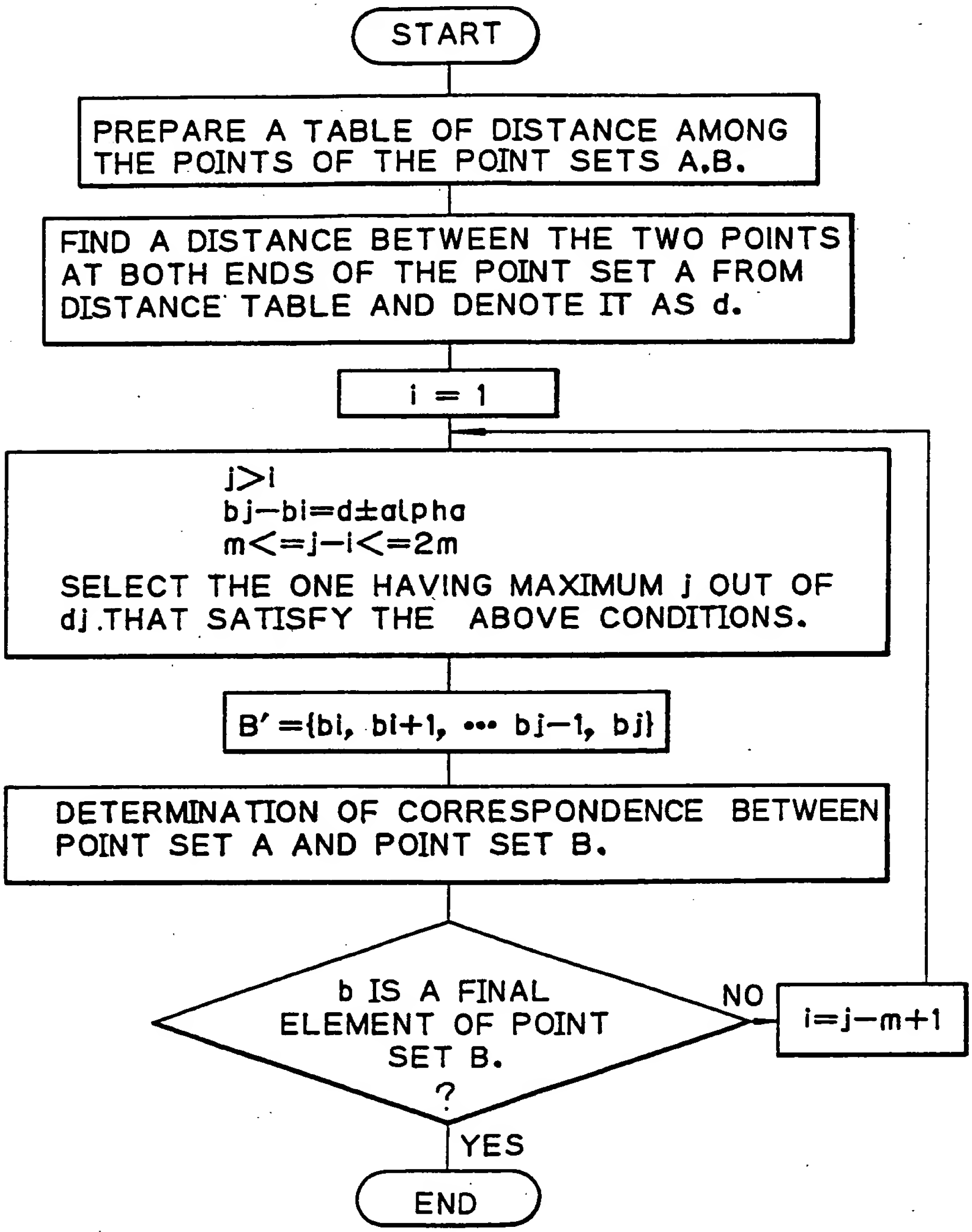

START
PREPARE A TABLE OF DISTANCE AMONG THE POINTS OF THE POINT SETS A.B.
FIND A DISTANCE BETWEEN THE TWO POINTS AT BOTH ENDS OF THE POINT SET A FROM DISTANCE TABLE AND DENOTE IT AS d.
i = 1
j>i
bj−bi=d±alpha
m<=j−i<=2m
SELECT THE ONE HAVING MAXIMUM j OUT OF dj THAT SATISFY THE ABOVE CONDITIONS.
B′={bi, bi+1, ••• bj−1, bj}
DETERMINATION OF CORRESPONDENCE BETWEEN POINT SET A AND POINT SET B.
b IS A FINAL ELEMENT OF POINT SET B. ?
NO
i=j−m+1
YES
END

Fig. 38 A

1	I V G G Y T C C A N	T V P Y Q V S L N S
21	G Y H F C G G S L I	N S Q W V V S A A H
41	C Y K S G I Q V R L	G E D N I N V V E G
61	N E Q F I S A S K S	I V H P S Y N S N T
81	L N N D I M L I K L	K S A A S L N S R V
101	A S I S L P T S C A	S A G T Q C L I S G
121	W G N T K S S G T S	Y P D V L K C L K A
141	P I L S D S S C K S	A Y P G Q I T S N M
161	F C A G Y L E G G K	D S C Q G D S G G P
181	V V C S G K L Q G I	V S W G S G C A Q K
201	N K P G V Y T K V C	N Y V S W I K Q T I
221	A S N	

AMINO ACID SEQUENCE OF TRYPSIN (EXCERPT FROM PDB)

Fig. 38 B

1	V V G G T E A Q R N	S W P S Q I S L Q Y
21	R S G S S W A H T C	G G T L I R Q N W V
41	M T A A H C V D R E	L T F R V V V G E H
61	N L N Q N N G T E Q	Y V G V Q K I V V
81	P Y W N T D D V A A	G Y D I A L L R L A
101	Q S V T L N S Y V Q	L G V L P R A G T I
121	L A N S P C Y I T T	G W G L T R T N G Q
141	L A Q T L Q Q A Y L	P T V D Y A I C S S
161	S S Y W G S T V K N	S M V C A G G D G V
181	R S G C Q G D S G G	P L H C L V N G Q Y
201	A V H G V T S F V S	R L G C N V T R K P
221	T V F T R V S A Y I	S W I N N V I A S N

AMINO ACID SEQUENCE OF ELASTASE (EXCERPT FROM PDB)

Fig. 39 A

```
Key site number 36 - 41 in Trypsin

41 42 43 44 45 46
 M  T  A  A  H  C   < target >
 V  S  A  A  H  C   < probe  >

d = 12.070038 [A]
r.m.s.d. = 0.061077 [A]
The number of atoms in a probe = 6
The number of atoms in PDB = 240
The number of combination = 1
Time = 1sec
```

RETRIEVED RESULTS OF HISTIDINE ACTIVE SITES

Fig. 39 B

```
Key site number 175 - 179 in Trypsin

186 187 188 189 190
  G   D   S   G   G   < target >
  G   D   S   G   G   < probe  >

d = 8.922721 [A]
r.m.s.d. = 0.092879 [A]
The number of atoms in a probe = 5
The number of atoms in PDB = 240
The number of combination = 1
Time = 1sec
```

RETRIEVED RESULTS OF SERINE ACTIVE SITES

Fig. 40

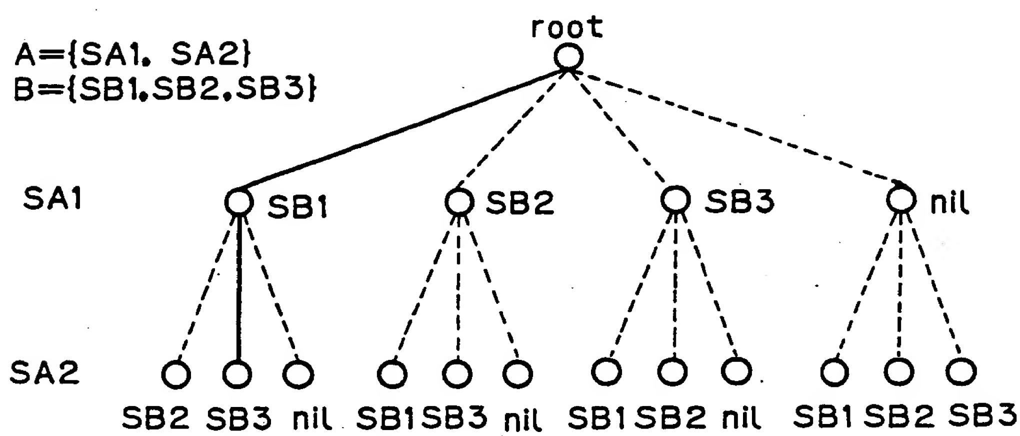

A={SA1, SA2}
B={SB1,SB2,SB3}
root
SA1
SB1
SB2
SB3
nil
SA2
SB2 SB3 nil SB1 SB3 nil SB1 SB2 nil SB1 SB2 SB3

Fig. 41

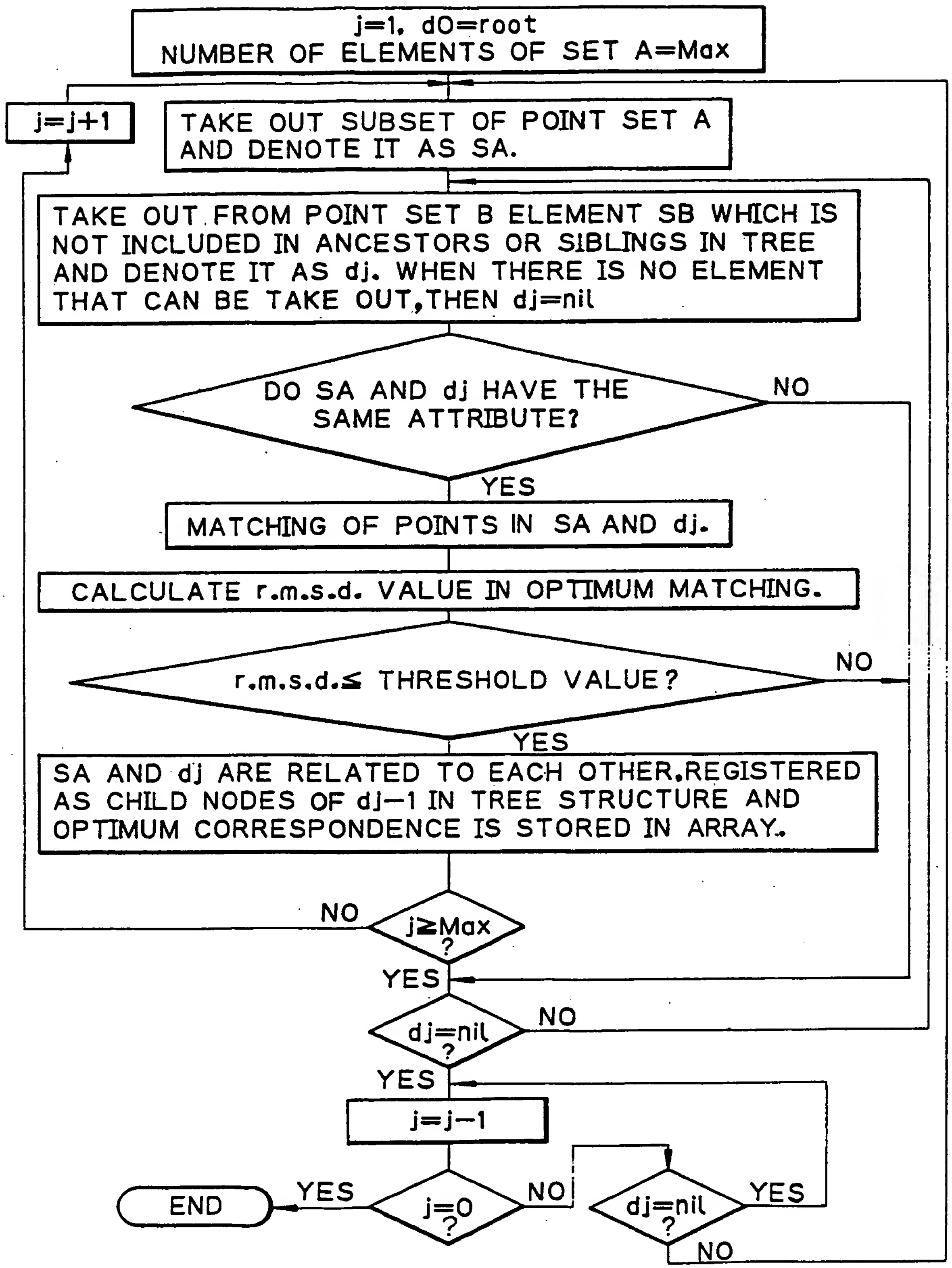

j=1, d0=root
NUMBER OF ELEMENTS OF SET A=Max
j=j+1
TAKE OUT SUBSET OF POINT SET A AND DENOTE IT AS SA.
TAKE OUT FROM POINT SET B ELEMENT SB WHICH IS NOT INCLUDED IN ANCESTORS OR SIBLINGS IN TREE AND DENOTE IT AS dj. WHEN THERE IS NO ELEMENT THAT CAN BE TAKE OUT,THEN dj=nil
DO SA AND dj HAVE THE SAME ATTRIBUTE?
NO
YES
MATCHING OF POINTS IN SA AND dj.
CALCULATE r.m.s.d. VALUE IN OPTIMUM MATCHING.
r.m.s.d.≤ THRESHOLD VALUE?
NO
YES
SA AND dj ARE RELATED TO EACH OTHER.REGISTERED AS CHILD NODES OF dj−1 IN TREE STRUCTURE AND OPTIMUM CORRESPONDENCE IS STORED IN ARRAY.
NO
j≥Max ?
YES
dj=nil ?
NO
YES
j=j−1
END
YES
j=0 ?
NO
dj=nil ?
YES
NO

Fig. 42

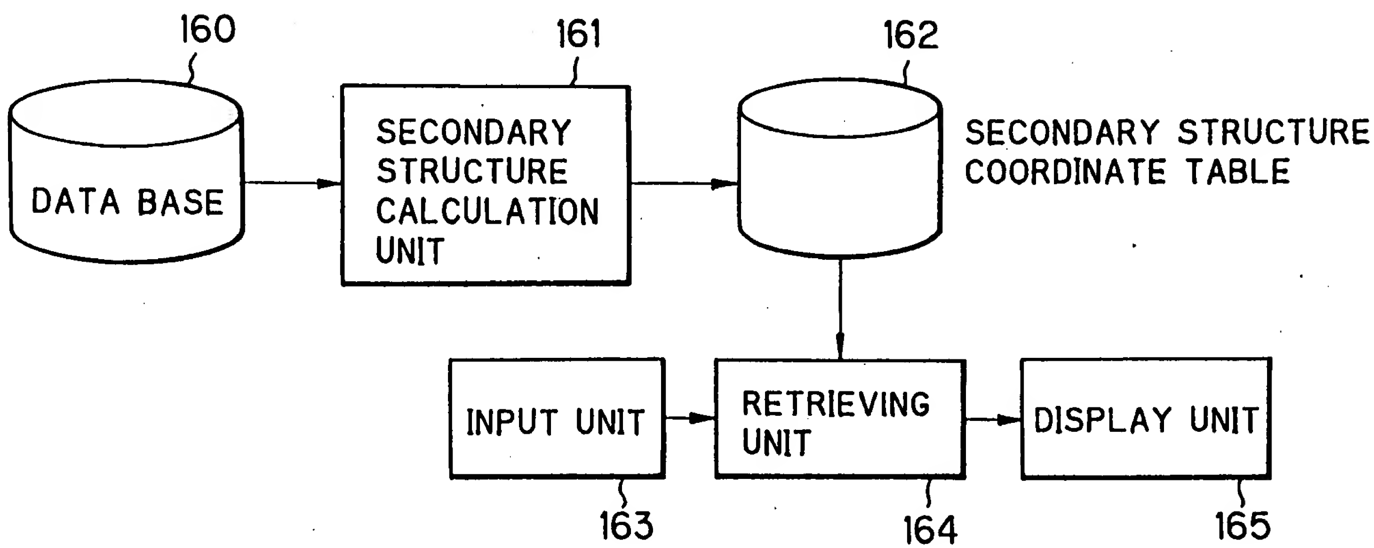

160
DATA BASE
161
SECONDARY STRUCTURE CALCULATION UNIT
162
SECONDARY STRUCTURE COORDINATE TABLE
INPUT UNIT
163
RETRIEVING UNIT
164
DISPLAY UNIT
165

Fig. 43

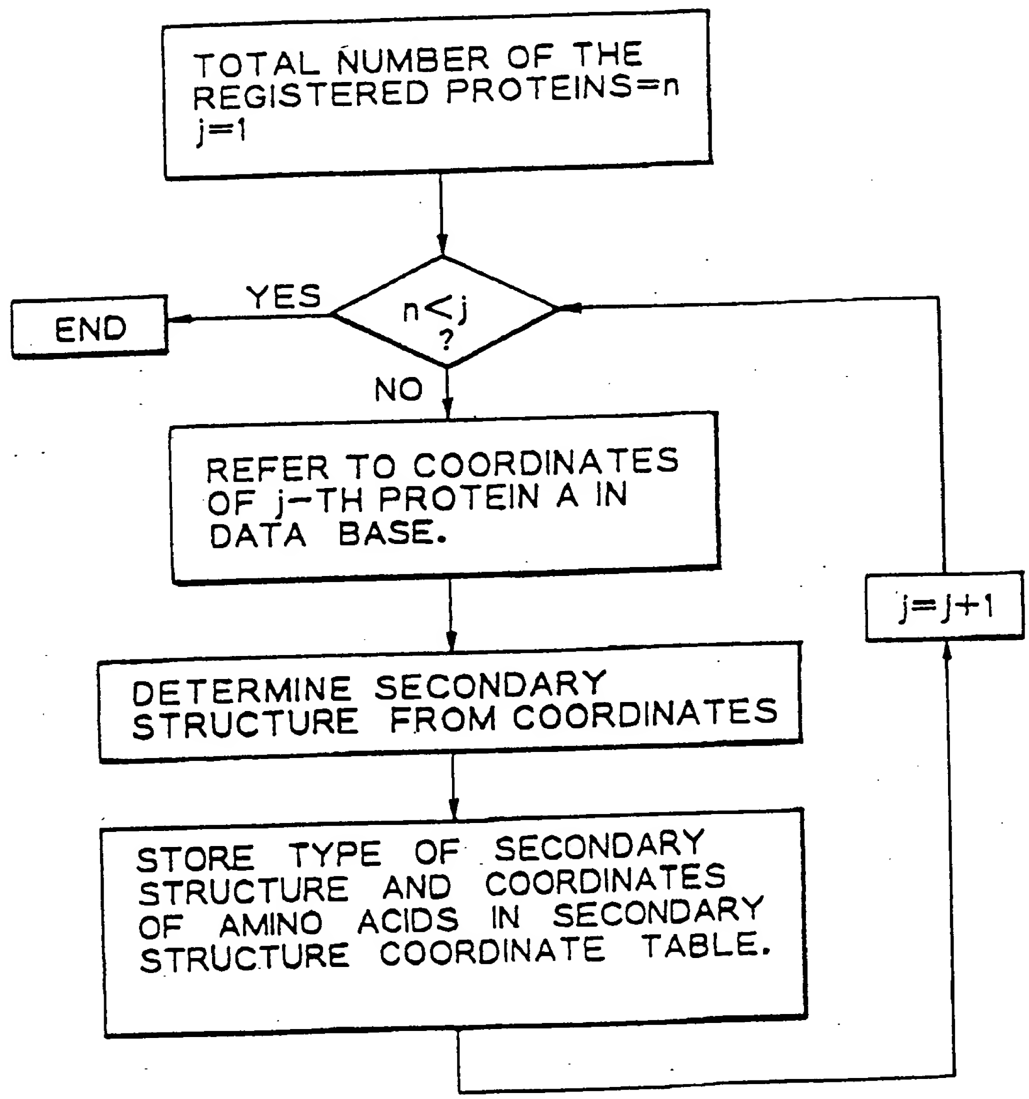

TOTAL NUMBER OF THE REGISTERED PROTEINS=n
j=1
n<j ?
YES
END
NO
REFER TO COORDINATES OF j-TH PROTEIN A IN DATA BASE.
DETERMINE SECONDARY STRUCTURE FROM COORDINATES
STORE TYPE OF SECONDARY STRUCTURE AND COORDINATES OF AMINO ACIDS IN SECONDARY STRUCTURE COORDINATE TABLE.
j=j+1

Fig. 44

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SUBSET	COORDINATES	TYPE
S1	$\{X1, X2, X3, X4, \cdots\cdots Xa\}$	α — HELIX
S2	$\{X_{a+1}, X_{a+2}, \cdots\cdots Xb\}$	α — HELIX
S3	$\{X_{b+1}, X_{b+2}, \cdots\cdots Xc\}$	β — SHEET
S4	$\{X_{c+1}, X_{c+2}, \cdots\cdots Xd\}$	β — SHEET
	⋮	⋮
Sn	$\{X_{l+1}, X_{l+2}, \cdots\cdots Xm\}$	3 — TURN

Fig. 45

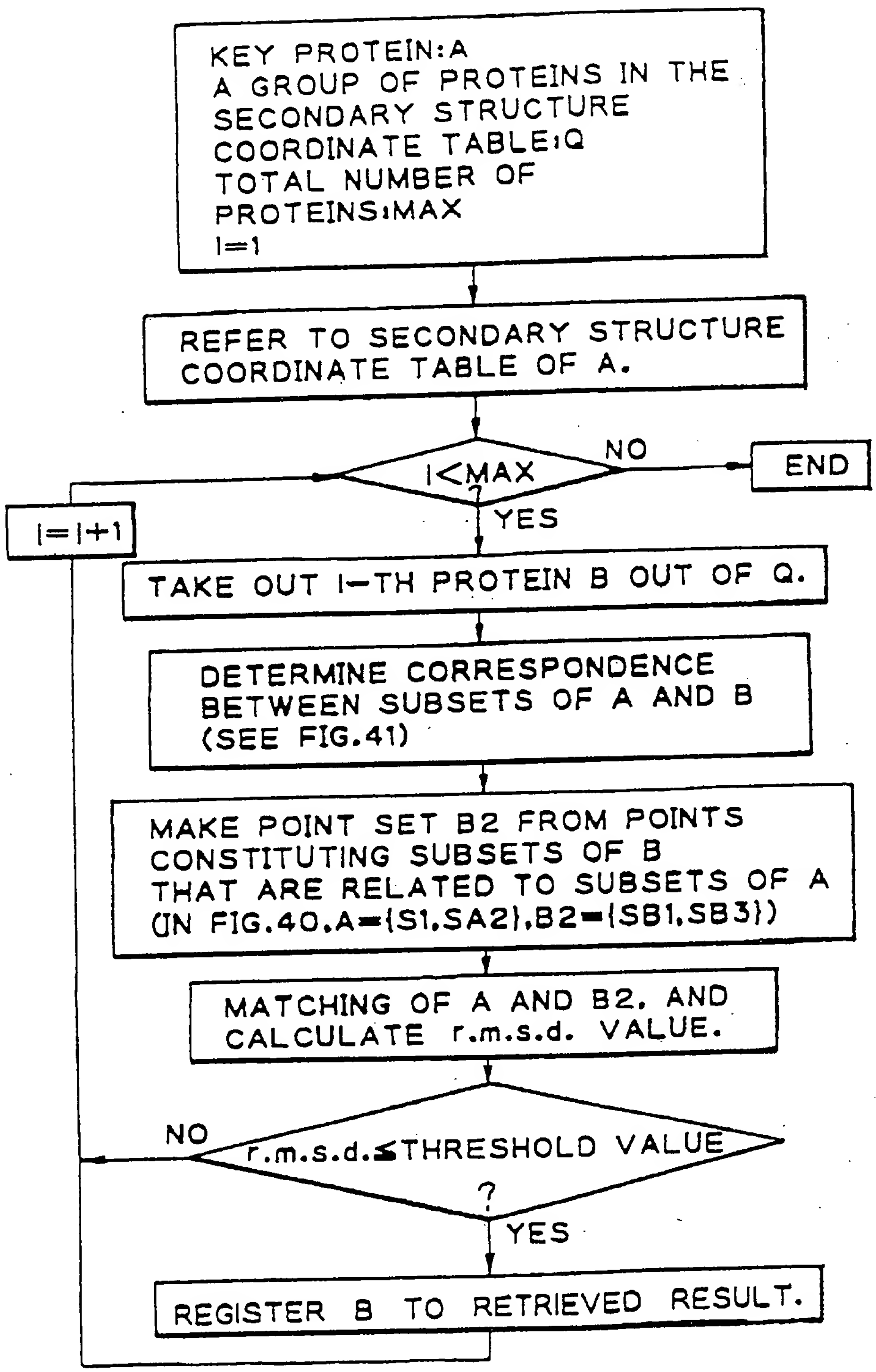

KEY PROTEIN:A
A GROUP OF PROTEINS IN THE SECONDARY STRUCTURE COORDINATE TABLE:Q
TOTAL NUMBER OF PROTEINS:MAX
I=1
REFER TO SECONDARY STRUCTURE COORDINATE TABLE OF A.
I<MAX ?
NO
END
YES
I=I+1
TAKE OUT I-TH PROTEIN B OUT OF Q.
DETERMINE CORRESPONDENCE BETWEEN SUBSETS OF A AND B (SEE FIG.41)
MAKE POINT SET B2 FROM POINTS CONSTITUTING SUBSETS OF B THAT ARE RELATED TO SUBSETS OF A (IN FIG.40.A={S1.SA2}.B2={SB1.SB3})
MATCHING OF A AND B2. AND CALCULATE r.m.s.d. VALUE.
NO
r.m.s.d.≤THRESHOLD VALUE ?
YES
REGISTER B TO RETRIEVED RESULT.

Fig. 46

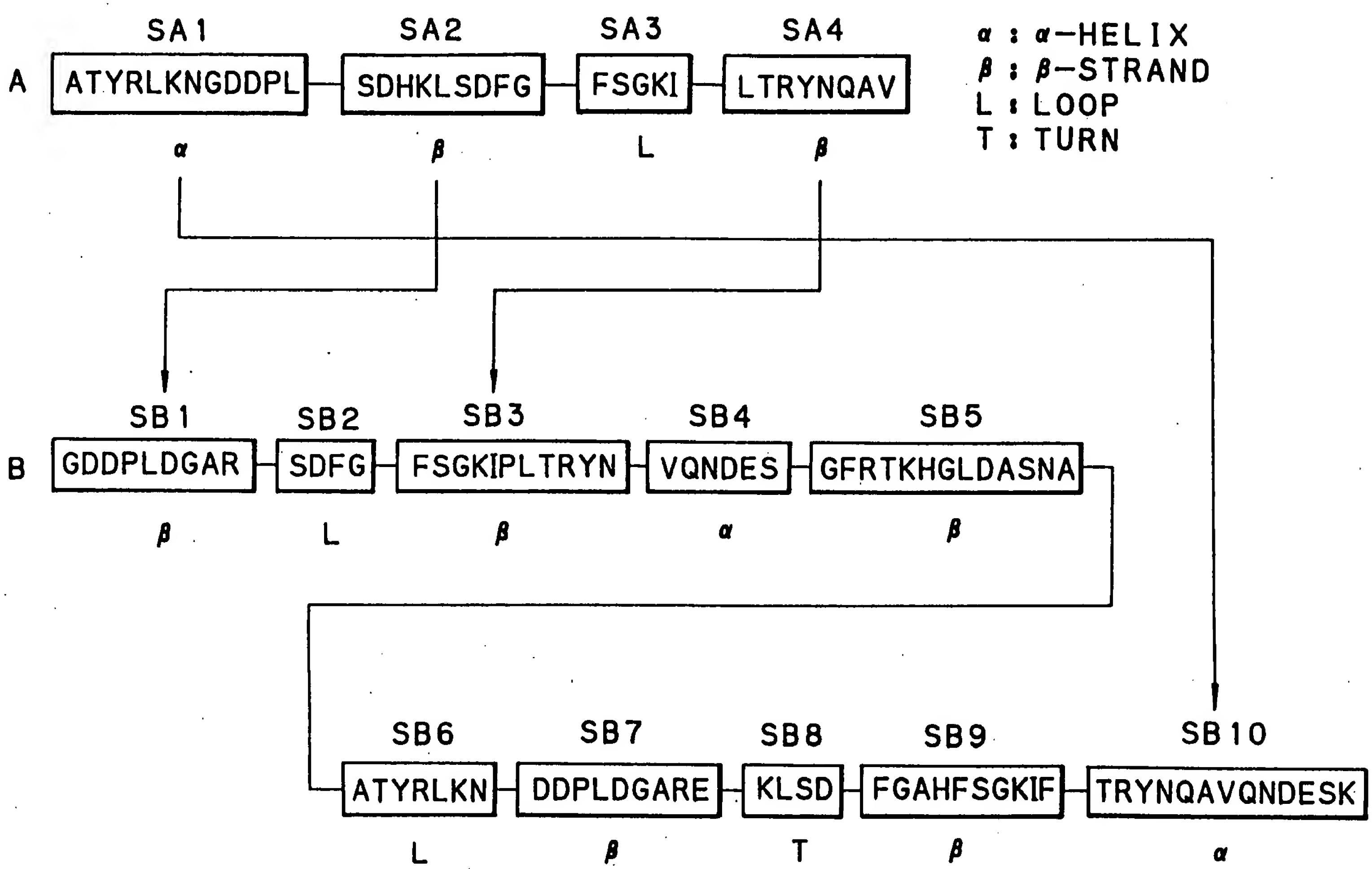
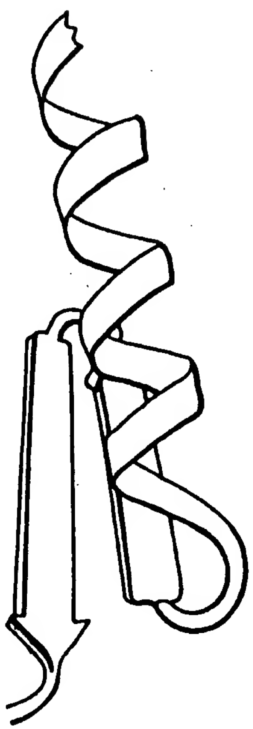
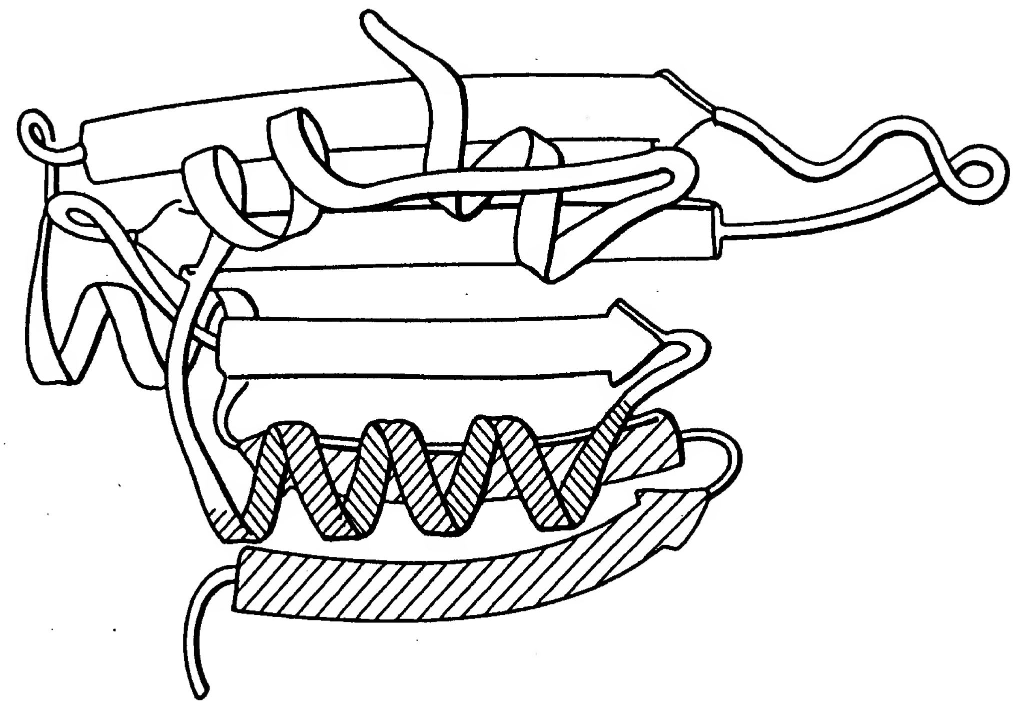

SA1
SA2
SA3
SA4
A
ATYRLKNGDDPL
SDHKLSDFG
FSGKI
LTRYNQAV
α
β
L
β
α : α-HELIX
β : β-STRAND
L : LOOP
T : TURN
SB1
SB2
SB3
SB4
SB5
B
GDDPLDGAR
SDFG
FSGKIPLTRYN
VQNDES
GFRTKHGLDASNA
β
L
β
α
β
SB6
SB7
SB8
SB9
SB10
ATYRLKN
DDPLDGARE
KLSD
FGAHFSGKIF
TRYNQAVQNDESK
L
β
T
β
α

Fig. 47 A



KEY PROTEIN A

Fig. 47 B



PROTEIN B HAVING A SIMILAR STRUCTURE